Entering Gaussian System, Link 0=g09

Input=ZnOMPC0td.com

Output=ZnOMPC0td.log

Initial command:

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

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

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

Gaussian, Inc. All Rights Reserved.

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

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

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

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

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

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

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

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

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

Carnegie Mellon University). Gaussian is a federally registered

trademark of Gaussian, Inc.

This software contains proprietary and confidential information,

including trade secrets, belonging to Gaussian, Inc.

This software is provided under written license and may be

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

written license.

The following legend is applicable only to US Government

contracts under FAR:

RESTRICTED RIGHTS LEGEND

Use, reproduction and disclosure by the US Government is

subject to restrictions as set forth in subparagraphs (a)

and (c) of the Commercial Computer Software - Restricted

Rights clause in FAR 52.227-19.

Gaussian, Inc.

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

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

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

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

assistance to any competitor of Gaussian, Inc. The licensee

of this program is prohibited from giving any competitor of

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

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

business of creating and licensing software in the field of

computational chemistry and represents and warrants to the

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

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

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

Cite this work as:

Gaussian 09, Revision E.01,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

19-Sep-2019

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

%nprocshared=9

Will use up to 9 processors via shared memory.

%mem=10GB

%chk=ZnOMPC0td.chk

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

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

ldispersion=gd3bj IOp(9/40=3)

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

1/38=1/1;

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

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

4//1;

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

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

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

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

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

Leave Link 1 at Thu Sep 19 00:35:41 2019, MaxMem= 1342177280 cpu: 0.4

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

---------

ZnOMPC0td

---------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C -1.12695 2.81013 0.01354

N 0. 2.04085 -0.0007

C 1.12695 2.81013 0.01354

C 0.70839 4.21655 0.04302

C -0.70839 4.21655 0.04302

N 2.39223 2.39223 0.

C 2.81013 1.12695 -0.01354

N 2.04085 0. 0.0007

C 2.81013 -1.12695 -0.01354

C 4.21655 -0.70839 -0.04302

C 4.21655 0.70839 -0.04302

N -2.39223 2.39223 0.

C -4.21655 0.70839 -0.04302

C -4.21655 -0.70839 -0.04302

C -2.81013 -1.12695 -0.01354

N -2.04085 0. 0.0007

C -2.81013 1.12695 -0.01354

N -2.39223 -2.39223 0.

N 0. -2.04085 -0.0007

C -1.12695 -2.81013 0.01354

C -0.70839 -4.21655 0.04302

C 0.70839 -4.21655 0.04302

C 1.12695 -2.81013 0.01354

N 2.39223 -2.39223 0.

Zn 0. 0. 0.

C -5.42079 1.43282 -0.07184

C -6.61032 0.6998 -0.09831

C -6.61032 -0.6998 -0.09831

C -5.42079 -1.43282 -0.07184

C 1.43282 -5.42079 0.07184

C 0.6998 -6.61032 0.09831

C -0.6998 -6.61032 0.09831

C -1.43282 -5.42079 0.07184

C 5.42079 1.43282 -0.07184

C 6.61032 0.6998 -0.09831

C 6.61032 -0.6998 -0.09831

C 5.42079 -1.43282 -0.07184

C -1.43282 5.42079 0.07184

C -0.6998 6.61032 0.09831

C 0.6998 6.61032 0.09831

C 1.43282 5.42079 0.07184

H 7.56515 1.20789 -0.12097

H 7.56515 -1.20789 -0.12097

H 1.20789 7.56515 0.12097

H -1.20789 7.56515 0.12097

H -7.56515 1.20789 -0.12097

H -7.56515 -1.20789 -0.12097

H -1.20789 -7.56515 0.12097

H 1.20789 -7.56515 0.12097

O 2.78394 5.3576 0.07395

O -2.78394 5.3576 0.07395

O 5.3576 2.78394 -0.07395

O 5.3576 -2.78394 -0.07395

O 2.78394 -5.3576 0.07395

O -2.78394 -5.3576 0.07395

O -5.3576 -2.78394 -0.07395

O -5.3576 2.78394 -0.07395

C 3.51435 6.58061 0.1027

H 3.30356 7.19436 -0.77851

H 4.56446 6.29392 0.09971

C 6.58061 3.51435 -0.1027

H 7.19436 3.30356 0.77851

H 6.29392 4.56446 -0.09971

C 6.58061 -3.51435 -0.1027

H 7.19436 -3.30356 0.77851

H 6.29392 -4.56446 -0.09971

C -3.51435 6.58061 0.1027

H -3.30356 7.19436 -0.77851

H -4.56446 6.29392 0.09971

C -6.58061 3.51435 -0.1027

H -7.19436 3.30356 0.77851

H -6.29392 4.56446 -0.09971

C -6.58061 -3.51435 -0.1027

H -7.19436 -3.30356 0.77851

H -6.29392 -4.56446 -0.09971

C -3.51435 -6.58061 0.1027

H -3.30356 -7.19436 -0.77851

H -4.56446 -6.29392 0.09971

C 3.51435 -6.58061 0.1027

H 3.30356 -7.19436 -0.77851

H 4.56446 -6.29392 0.09971

H 3.29834 -7.15574 1.00833

H -3.29834 -7.15574 1.00833

H -7.15574 -3.29834 -1.00833

H -7.15574 3.29834 -1.00833

H 3.29834 7.15574 1.00833

H -3.29834 7.15574 1.00833

H 7.15574 -3.29834 -1.00833

H 7.15574 3.29834 -1.00833

NAtoms= 89 NQM= 89 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

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

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

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

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

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

Atom 51 52 53 54 55 56 57 58 59 60

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

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

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

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

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

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

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

Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

Atom 71 72 73 74 75 76 77 78 79 80

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

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

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

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

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

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

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

Atom 81 82 83 84 85 86 87 88 89

IAtWgt= 1 1 1 1 1 1 1 1 1

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 1 1 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

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

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

Stoichiometry C40H32N8O8Zn

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

Deg. of freedom 32

Full point group D2D NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -1.126947 2.810131 0.013541

2 7 0 0.000000 2.040854 -0.000700

3 6 0 1.126947 2.810131 0.013541

4 6 0 0.708388 4.216552 0.043016

5 6 0 -0.708388 4.216552 0.043016

6 7 0 2.392227 2.392227 -0.000000

7 6 0 2.810131 1.126947 -0.013541

8 7 0 2.040854 -0.000000 0.000700

9 6 0 2.810131 -1.126947 -0.013541

10 6 0 4.216552 -0.708388 -0.043016

11 6 0 4.216552 0.708388 -0.043016

12 7 0 -2.392227 2.392227 -0.000000

13 6 0 -4.216552 0.708388 -0.043016

14 6 0 -4.216552 -0.708388 -0.043016

15 6 0 -2.810131 -1.126947 -0.013541

16 7 0 -2.040854 0.000000 0.000700

17 6 0 -2.810131 1.126947 -0.013541

18 7 0 -2.392227 -2.392227 -0.000000

19 7 0 -0.000000 -2.040854 -0.000700

20 6 0 -1.126947 -2.810131 0.013541

21 6 0 -0.708388 -4.216552 0.043016

22 6 0 0.708388 -4.216552 0.043016

23 6 0 1.126947 -2.810131 0.013541

24 7 0 2.392227 -2.392227 -0.000000

25 30 0 0.000000 0.000000 0.000000

26 6 0 -5.420785 1.432821 -0.071840

27 6 0 -6.610317 0.699802 -0.098313

28 6 0 -6.610317 -0.699802 -0.098313

29 6 0 -5.420785 -1.432821 -0.071840

30 6 0 1.432821 -5.420785 0.071840

31 6 0 0.699802 -6.610317 0.098313

32 6 0 -0.699802 -6.610317 0.098313

33 6 0 -1.432821 -5.420785 0.071840

34 6 0 5.420785 1.432821 -0.071840

35 6 0 6.610317 0.699802 -0.098313

36 6 0 6.610317 -0.699802 -0.098313

37 6 0 5.420785 -1.432821 -0.071840

38 6 0 -1.432821 5.420785 0.071840

39 6 0 -0.699802 6.610317 0.098313

40 6 0 0.699802 6.610317 0.098313

41 6 0 1.432821 5.420785 0.071840

42 1 0 7.565152 1.207886 -0.120969

43 1 0 7.565152 -1.207886 -0.120969

44 1 0 1.207886 7.565152 0.120969

45 1 0 -1.207886 7.565152 0.120969

46 1 0 -7.565152 1.207886 -0.120969

47 1 0 -7.565152 -1.207886 -0.120969

48 1 0 -1.207886 -7.565152 0.120969

49 1 0 1.207886 -7.565152 0.120969

50 8 0 2.783942 5.357598 0.073945

51 8 0 -2.783942 5.357598 0.073945

52 8 0 5.357598 2.783942 -0.073945

53 8 0 5.357598 -2.783942 -0.073945

54 8 0 2.783942 -5.357598 0.073945

55 8 0 -2.783942 -5.357598 0.073945

56 8 0 -5.357598 -2.783942 -0.073945

57 8 0 -5.357598 2.783942 -0.073945

58 6 0 3.514352 6.580615 0.102700

59 1 0 3.303559 7.194357 -0.778514

60 1 0 4.564460 6.293917 0.099713

61 6 0 6.580615 3.514352 -0.102700

62 1 0 7.194357 3.303559 0.778514

63 1 0 6.293917 4.564460 -0.099713

64 6 0 6.580615 -3.514352 -0.102700

65 1 0 7.194357 -3.303559 0.778514

66 1 0 6.293917 -4.564460 -0.099713

67 6 0 -3.514352 6.580615 0.102700

68 1 0 -3.303559 7.194357 -0.778514

69 1 0 -4.564460 6.293917 0.099713

70 6 0 -6.580615 3.514352 -0.102700

71 1 0 -7.194357 3.303559 0.778514

72 1 0 -6.293917 4.564460 -0.099713

73 6 0 -6.580615 -3.514352 -0.102700

74 1 0 -7.194357 -3.303559 0.778514

75 1 0 -6.293917 -4.564460 -0.099713

76 6 0 -3.514352 -6.580615 0.102700

77 1 0 -3.303559 -7.194357 -0.778514

78 1 0 -4.564460 -6.293917 0.099713

79 6 0 3.514352 -6.580615 0.102700

80 1 0 3.303559 -7.194357 -0.778514

81 1 0 4.564460 -6.293917 0.099713

82 1 0 3.298342 -7.155737 1.008335

83 1 0 -3.298342 -7.155737 1.008335

84 1 0 -7.155737 -3.298342 -1.008335

85 1 0 -7.155737 3.298342 -1.008335

86 1 0 3.298342 7.155737 1.008335

87 1 0 -3.298342 7.155737 1.008335

88 1 0 7.155737 -3.298342 -1.008335

89 1 0 7.155737 3.298342 -1.008335

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

Rotational constants (GHZ): 0.0443773 0.0443773 0.0222211

Leave Link 202 at Thu Sep 19 00:35:41 2019, MaxMem= 1342177280 cpu: 0.1

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

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

Centers: 25

S 1 1.00

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

S 1 1.00

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

S 1 1.00

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

P 1 1.00

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

P 1 1.00

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

D 3 1.00

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

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

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

D 1 1.00

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

D 1 1.00

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

\*\*\*\*

Centers: 42 43 44 45 46 47 48 49 59 60

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

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

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

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

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

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

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

Centers: 50 51 52 53 54 55 56 57

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 6

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 8

No pseudopotential on this center.

51 8

No pseudopotential on this center.

52 8

No pseudopotential on this center.

53 8

No pseudopotential on this center.

54 8

No pseudopotential on this center.

55 8

No pseudopotential on this center.

56 8

No pseudopotential on this center.

57 8

No pseudopotential on this center.

58 6

No pseudopotential on this center.

59 1

No pseudopotential on this center.

60 1

No pseudopotential on this center.

61 6

No pseudopotential on this center.

62 1

No pseudopotential on this center.

63 1

No pseudopotential on this center.

64 6

No pseudopotential on this center.

65 1

No pseudopotential on this center.

66 1

No pseudopotential on this center.

67 6

No pseudopotential on this center.

68 1

No pseudopotential on this center.

69 1

No pseudopotential on this center.

70 6

No pseudopotential on this center.

71 1

No pseudopotential on this center.

72 1

No pseudopotential on this center.

73 6

No pseudopotential on this center.

74 1

No pseudopotential on this center.

75 1

No pseudopotential on this center.

76 6

No pseudopotential on this center.

77 1

No pseudopotential on this center.

78 1

No pseudopotential on this center.

79 6

No pseudopotential on this center.

80 1

No pseudopotential on this center.

81 1

No pseudopotential on this center.

82 1

No pseudopotential on this center.

83 1

No pseudopotential on this center.

84 1

No pseudopotential on this center.

85 1

No pseudopotential on this center.

86 1

No pseudopotential on this center.

87 1

No pseudopotential on this center.

88 1

No pseudopotential on this center.

89 1

No pseudopotential on this center.

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

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

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

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

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

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

There are 295 symmetry adapted basis functions of A1 symmetry.

There are 271 symmetry adapted basis functions of A2 symmetry.

There are 281 symmetry adapted basis functions of B1 symmetry.

There are 281 symmetry adapted basis functions of B2 symmetry.

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

202 alpha electrons 202 beta electrons

nuclear repulsion energy 8035.3666833908 Hartrees.

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

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

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

NAtoms= 89 NActive= 89 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned on.

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

Nuclear repulsion after empirical dispersion term = 8035.1384609732 Hartrees.

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

Polarizable Continuum Model (PCM)

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

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

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : On-the-fly selection.

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

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 89.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

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

GePol: Number of generator spheres = 89

GePol: Total number of spheres = 89

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

GePol: Number of points = 6354

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.46D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 400

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

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

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

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

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

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

PCM non-electrostatic energy = -0.0073357608 Hartrees.

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

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

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

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

LDataN: DoStor=T MaxTD1= 5 Len= 102

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

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

Precomputing XC quadrature grid using

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

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

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

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

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

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

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

DipDrv: MaxL=1.

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

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

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

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

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

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

Petite list used in FoFCou.

Harris En= -2650.06149826476

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

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

LenX= 1339333041 LenY= 1337922885

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

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

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

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

IRaf= 450000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

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

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

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

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

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 121119948.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.01D-14 for 6349.

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

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

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

E= -2648.75788848665

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

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

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

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

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.082 Goal= None Shift= 0.000

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

Damping current iteration by 1.25D-01

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

Cycle 2 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

Coeff: -0.936D+00 0.194D+01

Gap= 0.073 Goal= None Shift= 0.000

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

Cycle 3 Pass 1 IDiag 1:

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

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

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

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

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

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

EnCoef did 100 forward-backward iterations

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

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

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

Gap= 0.071 Goal= None Shift= 0.000

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

Cycle 4 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.071 Goal= None Shift= 0.000

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

Cycle 5 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 6 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 7 Pass 1 IDiag 1:

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

CP: 6.63D-01

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

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

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

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

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

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

Coeff-Com: 0.481D+00

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

Coeff-En: 0.819D+00

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

Coeff: 0.482D+00

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 8 Pass 1 IDiag 1:

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

CP: 7.42D-01 6.39D-01

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

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

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

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

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

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

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

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

Coeff: 0.165D+00 0.727D+00

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 9 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

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

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

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 10 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

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

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

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 11 Pass 1 IDiag 1:

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

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

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

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

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

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

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

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

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

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

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

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 12 Pass 1 IDiag 1:

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

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

CP: 8.99D-01

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

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

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

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

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

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

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

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

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

Gap= 0.070 Goal= None Shift= 0.000

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

Cycle 13 Pass 1 IDiag 1:

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

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

CP: 9.05D-01 7.28D-01

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

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

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

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

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

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

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

Coeff-Com: 0.533D+00

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

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

Coeff: 0.533D+00

Gap= 0.070 Goal= None Shift= 0.000

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

Error on total polarization charges = 0.07340

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

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

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

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

(included in total energy above)

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

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

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

ExpMin= 3.51D-02 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

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

ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

Largest valence mixing into a core orbital is 5.14D-05

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

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

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

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

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

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

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

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

RHF ground state

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

Would need an additional 252071400000 words for in-memory AO integral storage.

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

Inv3: Mode=1 IEnd= 121119948.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.66D-15 for 6352.

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

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

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

Making orbital integer symmetry assigments:

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(A2)

40 initial guesses have been made.

Convergence on wavefunction: 0.001000000000000

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

Max sub-space: 200 roots to seek: 40 dimension of matrix: 270392

Iteration 1 Dimension 40 NMult 0 NNew 40

CISAX will form 40 AO SS matrices at one time.

NMat= 40 NSing= 40 JSym2X=-1.

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

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

New state 1 was old state 2

New state 2 was old state 1

New state 3 was old state 7

New state 4 was old state 6

New state 5 was old state 3

New state 6 was old state 4

New state 7 was old state 5

New state 9 was old state 12

New state 10 was old state 13

Excitation Energies [eV] at current iteration:

Root 1 : 1.900181167959592

Root 2 : 1.900181167962491

Root 3 : 2.484361198846707

Root 4 : 2.583202314384637

Root 5 : 2.600007276620242

Root 6 : 2.600007276626787

Root 7 : 2.692646640914146

Root 8 : 2.903190826581534

Root 9 : 3.133039755525036

Root 10 : 3.133039755525115

Root 11 : 3.272023548535302

Root 12 : 3.321641925066158

Root 13 : 3.321641925068831

Root 14 : 3.575335076057715

Root 15 : 3.575335076060520

Root 16 : 3.591708845242723

Root 17 : 3.591708845256204

Root 18 : 3.597090404400112

Root 19 : 3.611498540993447

Root 20 : 3.631857304973446

Root 21 : 3.641497150757556

Root 22 : 3.661601738624640

Root 23 : 3.679427398487915

Root 24 : 3.784492961789394

Root 25 : 3.823158333978653

Root 26 : 3.900212539688958

Root 27 : 3.900212539690033

Root 28 : 4.022220642153778

Root 29 : 4.022220642162383

Root 30 : 4.184368936600251

Root 31 : 4.205568621858740

Root 32 : 4.319135554485383

Root 33 : 4.319135554486715

Root 34 : 4.376219730551119

Root 35 : 4.376219730552508

Root 36 : 4.409177647231946

Root 37 : 4.799635976650545

Root 38 : 4.799635976650699

Root 39 : 5.020884230945949

Root 40 : 5.198377823645767

Iteration 2 Dimension 60 NMult 40 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.057231313645281

Root 2 not converged, maximum delta is 0.057231313644880

Root 3 not converged, maximum delta is 0.020269679046072

New state 4 was old state 5

Root 4 not converged, maximum delta is 0.049093039924765

New state 5 was old state 6

Root 5 not converged, maximum delta is 0.049093039922728

New state 6 was old state 4

Root 6 not converged, maximum delta is 0.050219065977987

Root 7 not converged, maximum delta is 0.065641748071347

Root 8 not converged, maximum delta is 0.102613532499864

Root 9 not converged, maximum delta is 0.392421749244570

Root 10 not converged, maximum delta is 0.392421749242944

Excitation Energies [eV] at current iteration:

Root 1 : 1.719166794607738 Change is -0.181014373351854

Root 2 : 1.719166794610989 Change is -0.181014373351501

Root 3 : 2.466419677395415 Change is -0.017941521451292

Root 4 : 2.496998476169038 Change is -0.103008800451204

Root 5 : 2.496998476177334 Change is -0.103008800449453

Root 6 : 2.507286167569716 Change is -0.075916146814921

Root 7 : 2.543048643823086 Change is -0.149597997091060

Root 8 : 2.665916903084227 Change is -0.237273923497308

Root 9 : 3.077962826907945 Change is -0.055076928617091

Root 10 : 3.077962826909841 Change is -0.055076928615274

Iteration 3 Dimension 80 NMult 60 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.017947308209105

Root 2 not converged, maximum delta is 0.017947308208187

Root 3 not converged, maximum delta is 0.002494424463759

Root 4 not converged, maximum delta is 0.006621684521004

Root 5 not converged, maximum delta is 0.006621684521185

Root 6 not converged, maximum delta is 0.006420946865318

Root 7 not converged, maximum delta is 0.051879899740317

Root 8 not converged, maximum delta is 0.011785879574896

Root 9 not converged, maximum delta is 0.010714193160829

Root 10 not converged, maximum delta is 0.010714193167414

Excitation Energies [eV] at current iteration:

Root 1 : 1.705030418556449 Change is -0.014136376051289

Root 2 : 1.705030418560499 Change is -0.014136376050490

Root 3 : 2.465642197857280 Change is -0.000777479538134

Root 4 : 2.492954181575997 Change is -0.004044294593040

Root 5 : 2.492954181584406 Change is -0.004044294592928

Root 6 : 2.504442458077695 Change is -0.002843709492021

Root 7 : 2.530021227200907 Change is -0.013027416622179

Root 8 : 2.654477217193296 Change is -0.011439685890931

Root 9 : 3.075977584626894 Change is -0.001985242281050

Root 10 : 3.075977584628204 Change is -0.001985242281637

Iteration 4 Dimension 100 NMult 80 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.011301101627306

Root 2 not converged, maximum delta is 0.011301101627295

Root 3 has converged.

Root 4 not converged, maximum delta is 0.002083397827316

Root 5 not converged, maximum delta is 0.002083397827773

Root 6 not converged, maximum delta is 0.003994277321353

Root 7 not converged, maximum delta is 0.003100540038221

Root 8 not converged, maximum delta is 0.003203379810082

Root 9 not converged, maximum delta is 0.005316419307843

Root 10 not converged, maximum delta is 0.005316419305105

Excitation Energies [eV] at current iteration:

Root 1 : 1.703735422937954 Change is -0.001294995618495

Root 2 : 1.703735422941958 Change is -0.001294995618541

Root 3 : 2.465516339827831 Change is -0.000125858029449

Root 4 : 2.492343270709044 Change is -0.000610910866952

Root 5 : 2.492343270717192 Change is -0.000610910867215

Root 6 : 2.503920463157269 Change is -0.000521994920426

Root 7 : 2.528718080662327 Change is -0.001303146538580

Root 8 : 2.653191803404130 Change is -0.001285413789165

Root 9 : 3.075704930226319 Change is -0.000272654400576

Root 10 : 3.075704930227816 Change is -0.000272654400388

Iteration 5 Dimension 118 NMult 100 NNew 18

CISAX will form 18 AO SS matrices at one time.

NMat= 18 NSing= 18 JSym2X=-1.

Root 1 not converged, maximum delta is 0.011300784358852

Root 2 not converged, maximum delta is 0.011300784358842

Root 3 has converged.

Root 4 has converged.

Root 5 has converged.

Root 6 has converged.

Root 7 has converged.

Root 8 has converged.

Root 9 not converged, maximum delta is 0.002742753269541

Root 10 not converged, maximum delta is 0.002742753265360

Excitation Energies [eV] at current iteration:

Root 1 : 1.703592254557351 Change is -0.000143168380603

Root 2 : 1.703592254561549 Change is -0.000143168380409

Root 3 : 2.465516339827864 Change is 0.000000000000033

Root 4 : 2.492302379000745 Change is -0.000040891708300

Root 5 : 2.492302379008794 Change is -0.000040891708398

Root 6 : 2.503860227245328 Change is -0.000060235911941

Root 7 : 2.528600019293039 Change is -0.000118061369288

Root 8 : 2.652996303208161 Change is -0.000195500195969

Root 9 : 3.075669241324304 Change is -0.000035688902015

Root 10 : 3.075669241325881 Change is -0.000035688901934

Iteration 6 Dimension 126 NMult 118 NNew 8

CISAX will form 8 AO SS matrices at one time.

NMat= 8 NSing= 8 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 has converged.

Root 4 has converged.

Root 5 has converged.

Root 6 has converged.

Root 7 has converged.

Root 8 has converged.

Root 9 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 1.703582990164302 Change is -0.000009264393049

Root 2 : 1.703582990168645 Change is -0.000009264392904

Root 3 : 2.465516339827864 Change is 0.000000000000000

Root 4 : 2.492301355074880 Change is -0.000001023925865

Root 5 : 2.492301355083126 Change is -0.000001023925667

Root 6 : 2.503860227245328 Change is 0.000000000000000

Root 7 : 2.528600019293039 Change is 0.000000000000000

Root 8 : 2.652996303208161 Change is 0.000000000000000

Root 9 : 3.075665165743650 Change is -0.000004075580654

Root 10 : 3.075665165745120 Change is -0.000004075580761

Convergence achieved on expansion vectors.

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

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

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

1PDM for each excited state written to RWF 633

Ground to excited state transition densities written to RWF 633

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

state X Y Z Dip. S. Osc.

1 -0.0000 4.0038 0.0000 16.0308 0.6691

2 -4.0038 -0.0000 -0.0000 16.0308 0.6691

3 -0.0000 0.0000 0.0000 0.0000 0.0000

4 -1.9979 0.0000 0.0000 3.9916 0.2437

5 -0.0000 -1.9979 -0.0000 3.9916 0.2437

6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

7 -0.0000 -0.0000 0.0590 0.0035 0.0002

8 0.0000 -0.0000 -0.0000 0.0000 0.0000

9 -0.1377 -0.0000 -0.0000 0.0189 0.0014

10 -0.0000 0.1377 0.0000 0.0189 0.0014

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

state X Y Z Dip. S. Osc.

1 0.0000 -0.2509 -0.0000 0.0630 0.6704

2 0.2509 0.0000 0.0000 0.0630 0.6704

3 0.0000 -0.0000 -0.0000 0.0000 0.0000

4 0.1806 -0.0000 -0.0000 0.0326 0.2373

5 0.0000 0.1806 0.0000 0.0326 0.2373

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 0.0000 0.0000 -0.0056 0.0000 0.0002

8 -0.0000 0.0000 -0.0000 0.0000 0.0000

9 0.0162 0.0000 0.0000 0.0003 0.0015

10 -0.0000 -0.0162 -0.0000 0.0003 0.0015

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

state X Y Z

1 -0.0126 0.0000 0.0000

2 0.0000 0.0126 0.0000

3 -0.0000 0.0000 1.2582

4 0.0000 0.0111 0.0000

5 0.0111 0.0000 0.0000

6 0.0000 0.0000 -0.0000

7 0.0000 -0.0000 -0.0000

8 0.0000 0.0000 -0.0000

9 0.0000 0.4245 0.0000

10 -0.4245 0.0000 0.0000

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

state XX YY ZZ XY XZ YZ

1 0.0000 -0.0000 -0.0000 0.0000 -0.0000 -0.0369

2 0.0000 0.0000 0.0000 -0.0000 -0.0369 0.0000

3 0.0000 -0.0000 0.0000 0.0000 -0.0000 -0.0000

4 0.0000 0.0000 0.0000 0.0000 -0.0435 -0.0000

5 -0.0000 0.0000 -0.0000 0.0000 -0.0000 0.0435

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

7 2.0536 -2.0536 -0.0000 0.0000 0.0000 0.0000

8 1.5007 1.5007 0.0100 -0.0000 -0.0000 0.0000

9 -0.0000 0.0000 -0.0000 0.0000 -0.1071 0.0000

10 0.0000 -0.0000 0.0000 0.0000 0.0000 -0.1071

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

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

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

1 -0.0000 -0.0000 0.0000 -0.0000 90.00

2 0.0000 0.0000 -0.0000 0.0000 90.00

3 -0.0000 -0.0000 0.0000 -0.0000 90.00

4 -0.0000 0.0000 0.0000 0.0000 90.00

5 0.0000 0.0000 -0.0000 0.0000 90.00

6 -0.0000 0.0000 -0.0000 -0.0000 90.00

7 0.0000 0.0000 -0.0000 0.0000 90.00

8 0.0000 0.0000 -0.0000 0.0000 90.00

9 0.0000 0.0000 0.0000 0.0000 90.00

10 -0.0000 0.0000 0.0000 0.0000 90.00

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

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

state XX YY ZZ R(length)

1 -0.0000 -0.0000 -0.0000 -0.0000

2 0.0000 0.0000 0.0000 0.0000

3 -0.0000 -0.0000 -0.0000 -0.0000

4 0.0000 -0.0000 -0.0000 0.0000

5 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 -0.0000 0.0000

7 0.0000 -0.0000 0.0000 0.0000

8 -0.0000 0.0000 -0.0000 -0.0000

9 0.0000 0.0000 0.0000 0.0000

10 -0.0000 -0.0000 -0.0000 -0.0000

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

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

1 -0.0000 -1.0046 -0.0000 1.0046 0.6697

2 -1.0046 -0.0000 -0.0000 1.0046 0.6697

3 -0.0000 -0.0000 -0.0000 0.0000 0.0000

4 -0.3607 -0.0000 -0.0000 0.3607 0.2405

5 -0.0000 -0.3607 -0.0000 0.3607 0.2405

6 -0.0000 -0.0000 -0.0000 0.0000 0.0000

7 -0.0000 -0.0000 -0.0003 0.0003 0.0002

8 -0.0000 -0.0000 0.0000 -0.0000 -0.0000

9 -0.0022 -0.0000 -0.0000 0.0022 0.0015

10 0.0000 -0.0022 -0.0000 0.0022 0.0015

Excitation energies and oscillator strengths:

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

71 -> 289 -0.00104

72 -> 282 -0.00106

90 -> 272 0.00115

97 -> 256 0.00109

101 -> 282 0.00107

102 -> 272 0.00107

105 -> 291 -0.00184

105 -> 334 -0.00128

110 -> 222 -0.00136

110 -> 227 0.00129

110 -> 246 0.00119

110 -> 272 -0.00103

111 -> 266 -0.00107

112 -> 291 0.00120

114 -> 225 0.00159

114 -> 229 -0.00100

115 -> 258 -0.00237

115 -> 265 0.00105

115 -> 272 0.00163

115 -> 287 -0.00212

116 -> 266 0.00212

116 -> 280 0.00115

116 -> 285 -0.00183

116 -> 288 -0.00103

116 -> 314 -0.00149

116 -> 389 0.00169

116 -> 402 0.00118

116 -> 435 0.00103

117 -> 232 0.00202

118 -> 230 0.00199

118 -> 235 0.00147

118 -> 236 0.00256

120 -> 228 -0.00116

120 -> 232 0.00198

120 -> 278 -0.00107

122 -> 216 -0.00102

122 -> 222 -0.00104

123 -> 230 0.00128

123 -> 266 0.00102

125 -> 220 -0.00155

125 -> 232 0.00132

125 -> 256 0.00114

125 -> 263 0.00116

125 -> 269 -0.00314

125 -> 278 0.00280

125 -> 301 -0.00128

125 -> 322 0.00105

125 -> 372 -0.00134

125 -> 443 -0.00115

126 -> 256 -0.00105

126 -> 274 -0.00117

127 -> 227 -0.00220

127 -> 234 -0.00148

127 -> 258 0.00135

127 -> 267 -0.00187

127 -> 275 0.00123

127 -> 293 0.00117

128 -> 230 0.00110

128 -> 254 0.00110

128 -> 257 -0.00108

129 -> 203 0.00131

129 -> 237 -0.00110

129 -> 247 0.00133

129 -> 318 -0.00124

130 -> 213 -0.00114

131 -> 205 0.00171

132 -> 203 -0.00150

133 -> 225 -0.00164

133 -> 229 0.00112

137 -> 204 -0.00109

138 -> 207 0.00178

138 -> 237 -0.00230

138 -> 239 -0.00114

138 -> 247 0.00102

138 -> 318 -0.00137

139 -> 228 -0.00151

139 -> 244 -0.00110

139 -> 256 0.00160

139 -> 263 0.00224

139 -> 269 0.00150

139 -> 274 -0.00173

139 -> 281 -0.00259

140 -> 218 0.00182

140 -> 222 -0.00174

140 -> 227 0.00122

140 -> 231 -0.00145

140 -> 234 -0.00180

140 -> 242 0.00144

140 -> 258 0.00257

140 -> 272 0.00101

141 -> 289 -0.00189

142 -> 224 -0.00128

142 -> 232 0.00100

142 -> 256 0.00127

142 -> 263 -0.00123

143 -> 206 -0.00303

143 -> 209 -0.00262

143 -> 213 -0.00289

143 -> 221 0.00232

143 -> 241 -0.00168

143 -> 253 -0.00144

143 -> 348 0.00114

144 -> 205 0.00232

144 -> 223 -0.00272

144 -> 260 -0.00125

145 -> 225 -0.00181

145 -> 229 0.00132

145 -> 243 -0.00191

145 -> 282 -0.00172

145 -> 284 0.00102

146 -> 217 -0.00250

146 -> 226 -0.00179

146 -> 235 0.00104

146 -> 254 0.00156

146 -> 257 -0.00150

146 -> 266 -0.00105

146 -> 270 0.00155

148 -> 214 0.00200

148 -> 224 -0.00169

148 -> 244 0.00105

148 -> 256 0.00154

148 -> 269 0.00103

149 -> 203 -0.00585

149 -> 207 0.00114

149 -> 212 -0.00160

149 -> 318 -0.00175

150 -> 215 -0.00154

150 -> 225 -0.00171

150 -> 243 -0.00234

150 -> 273 -0.00135

151 -> 216 -0.00297

151 -> 222 -0.00236

151 -> 231 -0.00114

151 -> 242 0.00274

151 -> 246 -0.00154

151 -> 265 0.00104

152 -> 217 0.00135

153 -> 215 0.00296

153 -> 219 -0.00126

153 -> 233 -0.00146

153 -> 243 0.00170

154 -> 239 0.00144

154 -> 243 -0.00205

155 -> 216 -0.00178

155 -> 234 0.00212

155 -> 246 0.00178

155 -> 258 0.00138

156 -> 235 0.00182

156 -> 257 0.00129

156 -> 266 0.00111

156 -> 285 -0.00116

156 -> 289 0.00194

157 -> 228 -0.00144

157 -> 244 -0.00102

157 -> 256 0.00168

157 -> 283 -0.00118

158 -> 226 0.00104

158 -> 230 -0.00109

158 -> 235 0.00155

158 -> 236 0.00117

158 -> 257 0.00117

158 -> 276 0.00148

158 -> 280 -0.00105

158 -> 289 -0.00189

158 -> 303 0.00124

158 -> 315 0.00118

158 -> 326 -0.00103

159 -> 218 0.00131

159 -> 246 0.00165

159 -> 258 0.00269

159 -> 267 -0.00116

159 -> 275 0.00151

159 -> 286 0.00121

160 -> 219 -0.00139

160 -> 239 0.00135

160 -> 268 -0.00130

160 -> 282 0.00252

160 -> 284 -0.00149

160 -> 302 -0.00113

160 -> 333 0.00120

161 -> 416 -0.00103

162 -> 204 0.00550

162 -> 208 -0.00168

162 -> 211 0.00194

162 -> 262 -0.00145

162 -> 319 -0.00131

162 -> 336 -0.00124

163 -> 204 0.00140

163 -> 240 0.00222

163 -> 263 0.00171

163 -> 274 -0.00266

163 -> 281 -0.00135

164 -> 203 0.00328

164 -> 207 -0.00137

164 -> 237 0.00121

164 -> 335 0.00181

165 -> 206 -0.00353

165 -> 209 -0.00221

165 -> 213 -0.00130

165 -> 221 0.00149

165 -> 241 -0.00123

165 -> 325 -0.00146

165 -> 327 -0.00150

165 -> 346 -0.00104

165 -> 348 0.00116

166 -> 223 -0.00152

167 -> 203 -0.00619

167 -> 207 0.00360

167 -> 212 -0.00230

167 -> 335 -0.00188

168 -> 209 0.00139

168 -> 221 -0.00101

169 -> 223 0.00196

169 -> 259 -0.00133

169 -> 339 0.00122

169 -> 357 -0.00156

170 -> 238 -0.00108

170 -> 354 -0.00119

171 -> 204 -0.00552

171 -> 208 0.00209

171 -> 211 -0.00296

172 -> 239 -0.00113

172 -> 243 -0.00122

172 -> 264 -0.00122

173 -> 254 -0.00116

173 -> 288 -0.00114

174 -> 218 -0.00161

174 -> 222 -0.00102

174 -> 231 0.00116

174 -> 234 -0.00146

174 -> 242 -0.00145

174 -> 265 -0.00196

174 -> 267 -0.00142

175 -> 225 0.00100

175 -> 239 -0.00156

175 -> 243 -0.00102

175 -> 264 -0.00127

176 -> 230 0.00102

176 -> 257 0.00140

176 -> 266 0.00234

176 -> 276 -0.00115

176 -> 285 -0.00297

176 -> 314 -0.00121

176 -> 343 0.00121

177 -> 216 -0.00215

177 -> 218 0.00651

177 -> 258 0.00353

177 -> 265 -0.00100

177 -> 267 0.00233

177 -> 272 -0.00106

177 -> 287 -0.00263

178 -> 256 -0.00257

178 -> 278 0.00192

179 -> 218 0.00461

179 -> 258 0.00110

179 -> 267 0.00115

179 -> 275 -0.00233

179 -> 287 -0.00220

180 -> 235 0.00118

180 -> 254 0.00276

180 -> 257 -0.00195

180 -> 266 0.00211

180 -> 276 0.00102

180 -> 288 0.00164

180 -> 314 -0.00211

181 -> 256 0.00264

181 -> 281 0.00212

181 -> 283 0.00136

181 -> 291 0.00134

182 -> 206 -0.00336

182 -> 209 0.00467

182 -> 213 0.00108

182 -> 221 0.00338

182 -> 271 0.00129

183 -> 205 0.00539

183 -> 210 -0.00544

183 -> 223 -0.00210

183 -> 259 0.00122

183 -> 339 -0.00163

183 -> 368 -0.00113

184 -> 203 -0.00463

184 -> 207 -0.00456

184 -> 212 -0.00252

184 -> 237 -0.00245

184 -> 239 -0.00123

184 -> 247 -0.00116

185 -> 203 -0.00116

185 -> 207 -0.00447

185 -> 212 -0.00406

185 -> 237 -0.00146

185 -> 247 -0.00199

185 -> 335 -0.00123

186 -> 206 0.00659

186 -> 209 0.00358

186 -> 213 -0.00273

186 -> 221 0.00220

186 -> 241 -0.00293

186 -> 245 -0.00232

186 -> 346 -0.00146

186 -> 348 0.00106

187 -> 205 0.00312

187 -> 210 -0.00282

187 -> 223 -0.00236

188 -> 233 0.00139

188 -> 268 -0.00159

188 -> 279 0.00207

188 -> 284 -0.00134

188 -> 292 0.00163

189 -> 216 -0.00115

189 -> 218 0.00389

189 -> 234 -0.00102

189 -> 265 0.00365

189 -> 271 -0.00162

189 -> 272 0.00602

189 -> 287 -0.00219

189 -> 293 0.00185

189 -> 310 -0.00171

190 -> 205 -0.00114

190 -> 230 0.00152

190 -> 266 0.00250

190 -> 285 -0.00236

190 -> 300 0.00115

190 -> 314 -0.00153

190 -> 324 -0.00107

190 -> 337 -0.00172

191 -> 203 0.00271

191 -> 215 0.00164

191 -> 219 0.00262

191 -> 233 -0.00144

191 -> 255 -0.00118

191 -> 264 -0.00183

191 -> 268 0.00441

191 -> 279 -0.00402

191 -> 282 0.00151

191 -> 284 -0.00255

191 -> 302 -0.00152

191 -> 309 -0.00192

191 -> 312 0.00259

191 -> 321 -0.00115

191 -> 353 -0.00125

191 -> 400 0.00101

191 -> 416 0.00141

192 -> 203 0.02474

192 -> 207 -0.00215

192 -> 212 -0.00175

192 -> 247 -0.00177

192 -> 261 -0.00220

192 -> 335 -0.00106

192 -> 355 0.00139

192 -> 363 -0.00144

193 -> 206 -0.00616

193 -> 209 -0.00860

193 -> 213 -0.00457

193 -> 221 0.00242

193 -> 241 -0.00224

193 -> 245 0.00115

193 -> 253 -0.00338

193 -> 271 -0.00151

193 -> 346 0.00166

193 -> 348 -0.00151

193 -> 375 -0.00122

194 -> 205 -0.00663

194 -> 210 -0.00549

194 -> 223 -0.00332

194 -> 259 0.00232

194 -> 260 -0.00294

195 -> 203 -0.00661

195 -> 207 0.00924

195 -> 212 -0.00479

195 -> 237 -0.00166

195 -> 247 0.00210

195 -> 261 -0.00227

195 -> 355 -0.00113

195 -> 363 0.00176

196 -> 203 -0.10434

196 -> 207 0.00643

196 -> 212 -0.01187

196 -> 261 -0.00198

197 -> 204 -0.00682

197 -> 220 0.00153

197 -> 263 -0.00231

197 -> 274 0.00240

197 -> 278 -0.00260

197 -> 283 0.00239

197 -> 291 -0.00374

197 -> 299 -0.00104

197 -> 301 -0.00129

197 -> 322 0.00108

198 -> 204 -0.03894

198 -> 208 -0.00637

198 -> 211 -0.00250

198 -> 238 0.00105

198 -> 248 -0.00129

198 -> 250 0.00204

198 -> 262 -0.00110

198 -> 354 0.00197

199 -> 205 -0.02850

199 -> 210 0.00998

199 -> 223 0.00346

199 -> 249 -0.00339

199 -> 252 -0.00310

199 -> 259 -0.00276

199 -> 357 0.00167

199 -> 368 0.00137

200 -> 206 -0.01057

200 -> 209 -0.00386

200 -> 213 0.00333

200 -> 221 0.01216

200 -> 241 0.00204

200 -> 245 0.00124

200 -> 253 0.00204

201 -> 204 0.03625

201 -> 208 -0.00378

201 -> 211 0.01051

201 -> 238 -0.00359

201 -> 240 -0.00174

201 -> 248 0.00238

201 -> 250 0.00391

201 -> 262 -0.00144

201 -> 354 0.00120

201 -> 364 0.00101

202 -> 204 0.70059

202 -> 208 -0.00145

202 -> 211 0.00160

202 -> 238 -0.00154

202 -> 250 -0.00300

202 -> 262 0.00181

202 -> 364 -0.00111

202 -> 381 -0.00209

202 -> 425 0.00114

90 <- 272 0.00107

105 <- 291 -0.00159

105 <- 334 -0.00113

110 <- 222 -0.00108

110 <- 227 0.00102

112 <- 291 0.00103

114 <- 225 0.00126

115 <- 258 -0.00202

115 <- 272 0.00145

115 <- 287 -0.00188

116 <- 266 0.00177

116 <- 280 0.00102

116 <- 285 -0.00155

116 <- 314 -0.00130

116 <- 389 0.00150

116 <- 402 0.00104

117 <- 232 0.00161

118 <- 230 0.00157

118 <- 235 0.00117

118 <- 236 0.00203

120 <- 232 0.00156

123 <- 230 0.00101

125 <- 220 -0.00124

125 <- 232 0.00107

125 <- 269 -0.00265

125 <- 278 0.00241

125 <- 301 -0.00111

125 <- 372 -0.00118

125 <- 443 -0.00103

127 <- 227 -0.00171

127 <- 234 -0.00117

127 <- 258 0.00111

127 <- 267 -0.00153

127 <- 275 0.00102

129 <- 203 0.00107

129 <- 247 0.00109

129 <- 318 -0.00108

133 <- 225 -0.00125

138 <- 207 0.00127

138 <- 237 -0.00190

138 <- 318 -0.00123

139 <- 228 -0.00117

139 <- 256 0.00128

139 <- 263 0.00186

139 <- 269 0.00123

139 <- 274 -0.00145

139 <- 281 -0.00219

140 <- 218 0.00134

140 <- 222 -0.00131

140 <- 231 -0.00112

140 <- 234 -0.00141

140 <- 242 0.00113

140 <- 258 0.00208

141 <- 289 -0.00160

142 <- 256 0.00101

143 <- 206 -0.00219

143 <- 209 -0.00191

143 <- 213 -0.00217

143 <- 221 0.00189

143 <- 241 -0.00153

143 <- 253 -0.00138

144 <- 205 0.00146

144 <- 223 -0.00192

145 <- 225 -0.00135

145 <- 243 -0.00149

145 <- 282 -0.00142

146 <- 217 -0.00187

146 <- 226 -0.00135

146 <- 254 0.00123

146 <- 257 -0.00118

146 <- 270 0.00124

148 <- 214 0.00149

148 <- 224 -0.00127

148 <- 256 0.00122

149 <- 203 -0.00305

149 <- 212 -0.00124

149 <- 318 -0.00143

150 <- 215 -0.00113

150 <- 225 -0.00127

150 <- 243 -0.00179

150 <- 273 -0.00109

151 <- 216 -0.00218

151 <- 222 -0.00174

151 <- 242 0.00210

151 <- 246 -0.00118

152 <- 217 0.00100

153 <- 215 0.00217

153 <- 233 -0.00111

153 <- 243 0.00130

154 <- 239 0.00107

154 <- 243 -0.00156

155 <- 216 -0.00129

155 <- 234 0.00157

155 <- 246 0.00134

155 <- 258 0.00113

156 <- 235 0.00137

156 <- 289 0.00158

157 <- 228 -0.00107

157 <- 256 0.00129

158 <- 235 0.00115

158 <- 276 0.00118

158 <- 289 -0.00160

158 <- 303 0.00103

159 <- 246 0.00124

159 <- 258 0.00214

159 <- 275 0.00123

160 <- 219 -0.00103

160 <- 268 -0.00107

160 <- 282 0.00206

160 <- 284 -0.00122

160 <- 333 0.00101

162 <- 204 0.00423

162 <- 211 0.00130

162 <- 238 0.00103

162 <- 262 -0.00112

162 <- 319 -0.00104

162 <- 336 -0.00104

163 <- 204 0.00107

163 <- 240 0.00174

163 <- 263 0.00137

163 <- 274 -0.00214

163 <- 281 -0.00112

164 <- 203 0.00269

164 <- 207 -0.00105

164 <- 237 0.00103

164 <- 335 0.00155

165 <- 206 -0.00258

165 <- 209 -0.00164

165 <- 221 0.00110

165 <- 241 -0.00109

165 <- 325 -0.00116

165 <- 327 -0.00125

165 <- 348 0.00103

166 <- 223 -0.00125

167 <- 203 -0.00268

167 <- 207 0.00284

167 <- 212 -0.00188

167 <- 335 -0.00151

168 <- 209 0.00119

169 <- 259 -0.00113

169 <- 357 -0.00132

170 <- 354 -0.00100

171 <- 204 -0.00438

171 <- 211 -0.00165

174 <- 218 -0.00112

174 <- 234 -0.00107

174 <- 242 -0.00106

174 <- 265 -0.00152

174 <- 267 -0.00110

175 <- 239 -0.00113

176 <- 257 0.00104

176 <- 266 0.00182

176 <- 285 -0.00236

176 <- 343 0.00100

177 <- 216 -0.00148

177 <- 218 0.00449

177 <- 258 0.00265

177 <- 267 0.00181

177 <- 287 -0.00209

178 <- 256 -0.00192

178 <- 278 0.00151

179 <- 218 0.00315

179 <- 275 -0.00186

179 <- 287 -0.00177

180 <- 254 0.00205

180 <- 257 -0.00145

180 <- 266 0.00161

180 <- 288 0.00129

180 <- 314 -0.00174

181 <- 256 0.00196

181 <- 281 0.00168

181 <- 283 0.00107

181 <- 291 0.00110

182 <- 206 -0.00160

182 <- 209 0.00279

182 <- 213 0.00103

182 <- 221 0.00117

182 <- 271 0.00124

183 <- 210 -0.00404

183 <- 339 -0.00120

184 <- 203 -0.00259

184 <- 207 -0.00247

184 <- 212 -0.00160

184 <- 237 -0.00178

185 <- 207 -0.00194

185 <- 212 -0.00265

185 <- 237 -0.00140

185 <- 247 -0.00109

185 <- 335 -0.00104

186 <- 206 0.00311

186 <- 209 0.00177

186 <- 213 -0.00183

186 <- 221 0.00212

186 <- 241 -0.00217

186 <- 245 -0.00150

186 <- 346 -0.00122

187 <- 210 -0.00205

188 <- 268 -0.00118

188 <- 279 0.00157

188 <- 284 -0.00105

188 <- 292 0.00129

189 <- 218 0.00248

189 <- 265 0.00273

189 <- 271 -0.00117

189 <- 272 0.00454

189 <- 287 -0.00173

189 <- 293 0.00148

189 <- 310 -0.00139

190 <- 230 0.00104

190 <- 266 0.00187

190 <- 285 -0.00181

190 <- 314 -0.00122

190 <- 337 -0.00141

191 <- 203 0.00143

191 <- 215 0.00104

191 <- 219 0.00167

191 <- 264 -0.00131

191 <- 268 0.00328

191 <- 279 -0.00306

191 <- 282 0.00111

191 <- 284 -0.00196

191 <- 302 -0.00120

191 <- 309 -0.00156

191 <- 312 0.00203

191 <- 353 -0.00100

191 <- 416 0.00120

192 <- 203 0.01295

192 <- 207 -0.00235

192 <- 212 -0.00142

192 <- 247 -0.00119

192 <- 261 -0.00184

192 <- 355 0.00120

192 <- 363 -0.00121

193 <- 206 -0.00495

193 <- 209 -0.00592

193 <- 213 -0.00264

193 <- 221 0.00173

193 <- 241 -0.00163

193 <- 253 -0.00233

193 <- 271 -0.00103

193 <- 346 0.00131

193 <- 348 -0.00122

193 <- 375 -0.00110

194 <- 205 -0.00449

194 <- 210 -0.00461

194 <- 223 -0.00211

194 <- 259 0.00216

194 <- 260 -0.00235

195 <- 203 -0.00268

195 <- 207 0.00671

195 <- 212 -0.00317

195 <- 237 -0.00136

195 <- 247 0.00153

195 <- 261 -0.00191

195 <- 363 0.00155

196 <- 203 -0.04613

196 <- 207 0.00554

196 <- 212 -0.00940

196 <- 261 -0.00205

197 <- 204 -0.00226

197 <- 263 -0.00169

197 <- 274 0.00179

197 <- 278 -0.00199

197 <- 283 0.00184

197 <- 291 -0.00293

197 <- 301 -0.00100

198 <- 204 -0.01838

198 <- 208 -0.00290

198 <- 211 -0.00353

198 <- 248 -0.00117

198 <- 250 0.00152

198 <- 354 0.00167

199 <- 205 -0.00222

199 <- 210 0.00430

199 <- 223 0.00172

199 <- 249 -0.00245

199 <- 252 -0.00234

199 <- 259 -0.00162

199 <- 357 0.00123

199 <- 368 0.00120

200 <- 206 -0.00199

200 <- 209 -0.00279

200 <- 213 0.00218

200 <- 221 0.00619

200 <- 241 0.00125

200 <- 253 0.00144

201 <- 204 0.01270

201 <- 208 0.00158

201 <- 211 0.00424

201 <- 238 -0.00166

201 <- 248 0.00115

201 <- 250 0.00273

202 <- 204 -0.07028

202 <- 211 -0.00180

202 <- 250 -0.00210

202 <- 381 -0.00179

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

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

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

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

70 -> 289 0.00104

72 -> 281 0.00106

91 -> 272 -0.00115

97 -> 255 -0.00109

101 -> 281 0.00107

103 -> 272 -0.00107

105 -> 292 0.00184

105 -> 333 -0.00128

110 -> 266 0.00107

111 -> 222 -0.00136

111 -> 227 -0.00129

111 -> 246 0.00119

111 -> 272 -0.00103

112 -> 292 -0.00120

114 -> 224 0.00159

114 -> 228 -0.00100

115 -> 266 -0.00212

115 -> 280 -0.00115

115 -> 285 0.00183

115 -> 288 -0.00103

115 -> 314 0.00149

115 -> 389 0.00169

115 -> 402 0.00118

115 -> 435 0.00103

116 -> 258 0.00237

116 -> 265 0.00105

116 -> 272 0.00163

116 -> 287 0.00212

117 -> 233 -0.00202

119 -> 230 -0.00199

119 -> 235 -0.00147

119 -> 236 0.00256

120 -> 229 -0.00116

120 -> 233 0.00198

120 -> 279 -0.00107

122 -> 230 -0.00128

122 -> 266 -0.00102

123 -> 216 0.00102

123 -> 222 -0.00104

125 -> 219 -0.00155

125 -> 233 0.00132

125 -> 255 0.00114

125 -> 264 0.00116

125 -> 268 -0.00314

125 -> 279 0.00280

125 -> 302 0.00128

125 -> 321 0.00105

125 -> 371 -0.00134

125 -> 444 -0.00115

126 -> 255 0.00105

126 -> 273 0.00117

127 -> 230 -0.00110

127 -> 254 -0.00110

127 -> 257 -0.00108

128 -> 227 0.00220

128 -> 234 0.00148

128 -> 258 -0.00135

128 -> 267 0.00187

128 -> 275 -0.00123

128 -> 293 0.00117

129 -> 204 -0.00131

129 -> 238 -0.00110

129 -> 248 0.00133

129 -> 319 0.00124

130 -> 205 -0.00171

131 -> 213 0.00114

132 -> 204 -0.00150

133 -> 224 0.00164

133 -> 228 -0.00112

137 -> 203 -0.00109

138 -> 208 -0.00178

138 -> 238 -0.00230

138 -> 240 -0.00114

138 -> 248 0.00102

138 -> 319 0.00137

139 -> 229 -0.00151

139 -> 243 -0.00110

139 -> 255 0.00160

139 -> 264 0.00224

139 -> 268 0.00150

139 -> 273 -0.00173

139 -> 282 -0.00259

140 -> 289 0.00189

141 -> 218 -0.00182

141 -> 222 -0.00174

141 -> 227 -0.00122

141 -> 231 -0.00145

141 -> 234 0.00180

141 -> 242 -0.00144

141 -> 258 -0.00257

141 -> 272 0.00101

142 -> 225 0.00128

142 -> 233 -0.00100

142 -> 255 -0.00127

142 -> 264 0.00123

143 -> 205 -0.00232

143 -> 223 0.00272

143 -> 260 0.00125

144 -> 206 -0.00303

144 -> 209 0.00262

144 -> 213 0.00289

144 -> 221 0.00232

144 -> 241 0.00168

144 -> 253 0.00144

144 -> 348 -0.00114

145 -> 224 -0.00181

145 -> 228 0.00132

145 -> 244 -0.00191

145 -> 281 -0.00172

145 -> 283 0.00102

147 -> 217 0.00250

147 -> 226 -0.00179

147 -> 235 -0.00104

147 -> 254 -0.00156

147 -> 257 -0.00150

147 -> 266 0.00105

147 -> 270 0.00155

148 -> 215 0.00200

148 -> 225 -0.00169

148 -> 243 0.00105

148 -> 255 0.00154

148 -> 268 0.00103

149 -> 204 -0.00585

149 -> 208 0.00114

149 -> 211 -0.00160

149 -> 319 -0.00175

150 -> 214 0.00154

150 -> 224 0.00171

150 -> 244 0.00234

150 -> 274 0.00135

151 -> 217 -0.00135

152 -> 216 0.00297

152 -> 222 -0.00236

152 -> 231 -0.00114

152 -> 242 -0.00274

152 -> 246 -0.00154

152 -> 265 0.00104

153 -> 214 0.00296

153 -> 220 -0.00126

153 -> 232 -0.00146

153 -> 244 0.00170

154 -> 240 -0.00144

154 -> 244 0.00205

155 -> 235 0.00182

155 -> 257 -0.00129

155 -> 266 0.00111

155 -> 285 -0.00116

155 -> 289 0.00194

156 -> 216 -0.00178

156 -> 234 0.00212

156 -> 246 -0.00178

156 -> 258 0.00138

157 -> 229 0.00144

157 -> 243 0.00102

157 -> 255 -0.00168

157 -> 284 0.00118

158 -> 218 -0.00131

158 -> 246 0.00165

158 -> 258 -0.00269

158 -> 267 0.00116

158 -> 275 -0.00151

158 -> 286 0.00121

159 -> 226 0.00104

159 -> 230 0.00109

159 -> 235 -0.00155

159 -> 236 0.00117

159 -> 257 0.00117

159 -> 276 0.00148

159 -> 280 0.00105

159 -> 289 0.00189

159 -> 303 -0.00124

159 -> 315 0.00118

159 -> 326 0.00103

160 -> 220 -0.00139

160 -> 240 0.00135

160 -> 269 -0.00130

160 -> 281 0.00252

160 -> 283 -0.00149

160 -> 301 0.00113

160 -> 334 -0.00120

161 -> 417 0.00103

162 -> 203 -0.00550

162 -> 207 0.00168

162 -> 212 -0.00194

162 -> 261 -0.00145

162 -> 318 0.00131

162 -> 335 0.00124

163 -> 203 -0.00140

163 -> 239 0.00222

163 -> 264 0.00171

163 -> 273 -0.00266

163 -> 282 -0.00135

164 -> 204 -0.00328

164 -> 208 0.00137

164 -> 238 0.00121

164 -> 336 -0.00181

165 -> 223 0.00152

166 -> 206 -0.00353

166 -> 209 0.00221

166 -> 213 0.00130

166 -> 221 0.00149

166 -> 241 0.00123

166 -> 325 -0.00146

166 -> 327 0.00150

166 -> 346 -0.00104

166 -> 348 -0.00116

167 -> 204 -0.00619

167 -> 208 0.00360

167 -> 211 -0.00230

167 -> 336 -0.00188

168 -> 223 -0.00196

168 -> 259 -0.00133

168 -> 339 -0.00122

168 -> 357 -0.00156

169 -> 209 -0.00139

169 -> 221 -0.00101

170 -> 237 0.00108

170 -> 355 -0.00119

171 -> 203 0.00552

171 -> 207 -0.00209

171 -> 212 0.00296

172 -> 240 0.00113

172 -> 244 0.00122

172 -> 263 0.00122

173 -> 218 0.00161

173 -> 222 -0.00102

173 -> 231 0.00116

173 -> 234 0.00146

173 -> 242 0.00145

173 -> 265 -0.00196

173 -> 267 0.00142

174 -> 254 0.00116

174 -> 288 -0.00114

175 -> 224 0.00100

175 -> 240 -0.00156

175 -> 244 -0.00102

175 -> 263 -0.00127

176 -> 216 0.00215

176 -> 218 -0.00651

176 -> 258 -0.00353

176 -> 265 -0.00100

176 -> 267 -0.00233

176 -> 272 -0.00106

176 -> 287 0.00263

177 -> 230 -0.00102

177 -> 257 0.00140

177 -> 266 -0.00234

177 -> 276 -0.00115

177 -> 285 0.00297

177 -> 314 0.00121

177 -> 343 -0.00121

178 -> 255 0.00257

178 -> 279 -0.00192

179 -> 235 -0.00118

179 -> 254 -0.00276

179 -> 257 -0.00195

179 -> 266 -0.00211

179 -> 276 0.00102

179 -> 288 0.00164

179 -> 314 0.00211

180 -> 218 -0.00461

180 -> 258 -0.00110

180 -> 267 -0.00115

180 -> 275 0.00233

180 -> 287 0.00220

181 -> 255 0.00264

181 -> 282 0.00212

181 -> 284 0.00136

181 -> 292 0.00134

182 -> 205 0.00539

182 -> 210 0.00544

182 -> 223 -0.00210

182 -> 259 -0.00122

182 -> 339 -0.00163

182 -> 368 -0.00113

183 -> 206 0.00336

183 -> 209 0.00467

183 -> 213 0.00108

183 -> 221 -0.00338

183 -> 271 0.00129

184 -> 204 0.00463

184 -> 208 0.00456

184 -> 211 0.00252

184 -> 238 -0.00245

184 -> 240 -0.00123

184 -> 248 -0.00116

185 -> 204 -0.00116

185 -> 208 -0.00447

185 -> 211 -0.00406

185 -> 238 0.00146

185 -> 248 0.00199

185 -> 336 -0.00123

186 -> 205 -0.00312

186 -> 210 -0.00282

186 -> 223 0.00236

187 -> 206 0.00659

187 -> 209 -0.00358

187 -> 213 0.00273

187 -> 221 0.00220

187 -> 241 0.00293

187 -> 245 -0.00232

187 -> 346 -0.00146

187 -> 348 -0.00106

188 -> 232 -0.00139

188 -> 269 0.00159

188 -> 278 -0.00207

188 -> 283 0.00134

188 -> 291 -0.00163

189 -> 205 -0.00114

189 -> 230 -0.00152

189 -> 266 -0.00250

189 -> 285 0.00236

189 -> 300 0.00115

189 -> 314 0.00153

189 -> 324 -0.00107

189 -> 337 -0.00172

190 -> 216 0.00115

190 -> 218 -0.00389

190 -> 234 0.00102

190 -> 265 0.00365

190 -> 271 -0.00162

190 -> 272 0.00602

190 -> 287 0.00219

190 -> 293 0.00185

190 -> 310 -0.00171

191 -> 204 -0.00271

191 -> 214 0.00164

191 -> 220 0.00262

191 -> 232 -0.00144

191 -> 256 -0.00118

191 -> 263 -0.00183

191 -> 269 0.00441

191 -> 278 -0.00402

191 -> 281 0.00151

191 -> 283 -0.00255

191 -> 301 0.00152

191 -> 308 -0.00192

191 -> 313 0.00259

191 -> 322 -0.00115

191 -> 352 -0.00125

191 -> 401 0.00101

191 -> 417 0.00141

192 -> 204 -0.02474

192 -> 208 0.00215

192 -> 211 0.00175

192 -> 248 -0.00177

192 -> 262 -0.00220

192 -> 336 0.00106

192 -> 354 -0.00139

192 -> 364 0.00144

193 -> 205 0.00663

193 -> 210 -0.00549

193 -> 223 0.00332

193 -> 259 0.00232

193 -> 260 0.00294

194 -> 206 -0.00616

194 -> 209 0.00860

194 -> 213 0.00457

194 -> 221 0.00242

194 -> 241 0.00224

194 -> 245 0.00115

194 -> 253 0.00338

194 -> 271 0.00151

194 -> 346 0.00166

194 -> 348 0.00151

194 -> 375 0.00122

195 -> 204 -0.00661

195 -> 208 0.00924

195 -> 211 -0.00479

195 -> 238 0.00166

195 -> 248 -0.00210

195 -> 262 0.00227

195 -> 354 -0.00113

195 -> 364 0.00176

196 -> 204 0.10434

196 -> 208 -0.00643

196 -> 211 0.01187

196 -> 262 -0.00198

197 -> 203 -0.00682

197 -> 219 -0.00153

197 -> 264 0.00231

197 -> 273 -0.00240

197 -> 279 0.00260

197 -> 284 -0.00239

197 -> 292 0.00374

197 -> 298 0.00104

197 -> 302 -0.00129

197 -> 321 -0.00108

198 -> 203 -0.03894

198 -> 207 -0.00637

198 -> 212 -0.00250

198 -> 237 -0.00105

198 -> 247 0.00129

198 -> 251 0.00204

198 -> 261 0.00110

198 -> 355 0.00197

199 -> 206 -0.01057

199 -> 209 0.00386

199 -> 213 -0.00333

199 -> 221 0.01216

199 -> 241 -0.00204

199 -> 245 0.00124

199 -> 253 -0.00204

200 -> 205 0.02850

200 -> 210 0.00998

200 -> 223 -0.00346

200 -> 249 0.00339

200 -> 252 -0.00310

200 -> 259 -0.00276

200 -> 357 0.00167

200 -> 368 -0.00137

201 -> 203 -0.03625

201 -> 207 0.00378

201 -> 212 -0.01051

201 -> 237 -0.00359

201 -> 239 -0.00174

201 -> 247 0.00238

201 -> 251 -0.00391

201 -> 261 -0.00144

201 -> 355 -0.00120

201 -> 363 -0.00101

202 -> 203 0.70059

202 -> 207 -0.00145

202 -> 212 0.00160

202 -> 237 0.00154

202 -> 251 -0.00300

202 -> 261 -0.00181

202 -> 363 -0.00111

202 -> 380 -0.00209

202 -> 424 0.00114

91 <- 272 -0.00107

105 <- 292 0.00159

105 <- 333 -0.00113

111 <- 222 -0.00108

111 <- 227 -0.00102

112 <- 292 -0.00103

114 <- 224 0.00126

115 <- 266 -0.00177

115 <- 280 -0.00102

115 <- 285 0.00155

115 <- 314 0.00130

115 <- 389 0.00150

115 <- 402 0.00104

116 <- 258 0.00202

116 <- 272 0.00145

116 <- 287 0.00188

117 <- 233 -0.00161

119 <- 230 -0.00157

119 <- 235 -0.00117

119 <- 236 0.00203

120 <- 233 0.00156

122 <- 230 -0.00101

125 <- 219 -0.00124

125 <- 233 0.00107

125 <- 268 -0.00265

125 <- 279 0.00241

125 <- 302 0.00111

125 <- 371 -0.00118

125 <- 444 -0.00103

128 <- 227 0.00171

128 <- 234 0.00117

128 <- 258 -0.00111

128 <- 267 0.00153

128 <- 275 -0.00102

129 <- 204 -0.00107

129 <- 248 0.00109

129 <- 319 0.00108

133 <- 224 0.00125

138 <- 208 -0.00127

138 <- 238 -0.00190

138 <- 319 0.00123

139 <- 229 -0.00117

139 <- 255 0.00128

139 <- 264 0.00186

139 <- 268 0.00123

139 <- 273 -0.00145

139 <- 282 -0.00219

140 <- 289 0.00160

141 <- 218 -0.00134

141 <- 222 -0.00131

141 <- 231 -0.00112

141 <- 234 0.00141

141 <- 242 -0.00113

141 <- 258 -0.00208

142 <- 255 -0.00101

143 <- 205 -0.00146

143 <- 223 0.00192

144 <- 206 -0.00219

144 <- 209 0.00191

144 <- 213 0.00217

144 <- 221 0.00189

144 <- 241 0.00153

144 <- 253 0.00138

145 <- 224 -0.00135

145 <- 244 -0.00149

145 <- 281 -0.00142

147 <- 217 0.00187

147 <- 226 -0.00135

147 <- 254 -0.00123

147 <- 257 -0.00118

147 <- 270 0.00124

148 <- 215 0.00149

148 <- 225 -0.00127

148 <- 255 0.00122

149 <- 204 -0.00305

149 <- 211 -0.00124

149 <- 319 -0.00143

150 <- 214 0.00113

150 <- 224 0.00127

150 <- 244 0.00179

150 <- 274 0.00109

151 <- 217 -0.00100

152 <- 216 0.00218

152 <- 222 -0.00174

152 <- 242 -0.00210

152 <- 246 -0.00118

153 <- 214 0.00217

153 <- 232 -0.00111

153 <- 244 0.00130

154 <- 240 -0.00107

154 <- 244 0.00156

155 <- 235 0.00137

155 <- 289 0.00158

156 <- 216 -0.00129

156 <- 234 0.00157

156 <- 246 -0.00134

156 <- 258 0.00113

157 <- 229 0.00107

157 <- 255 -0.00129

158 <- 246 0.00124

158 <- 258 -0.00214

158 <- 275 -0.00123

159 <- 235 -0.00115

159 <- 276 0.00118

159 <- 289 0.00160

159 <- 303 -0.00103

160 <- 220 -0.00103

160 <- 269 -0.00107

160 <- 281 0.00206

160 <- 283 -0.00122

160 <- 334 -0.00101

162 <- 203 -0.00423

162 <- 212 -0.00130

162 <- 237 0.00103

162 <- 261 -0.00112

162 <- 318 0.00104

162 <- 335 0.00104

163 <- 203 -0.00107

163 <- 239 0.00174

163 <- 264 0.00137

163 <- 273 -0.00214

163 <- 282 -0.00112

164 <- 204 -0.00269

164 <- 208 0.00105

164 <- 238 0.00103

164 <- 336 -0.00155

165 <- 223 0.00125

166 <- 206 -0.00258

166 <- 209 0.00164

166 <- 221 0.00110

166 <- 241 0.00109

166 <- 325 -0.00116

166 <- 327 0.00125

166 <- 348 -0.00103

167 <- 204 -0.00268

167 <- 208 0.00284

167 <- 211 -0.00188

167 <- 336 -0.00151

168 <- 259 -0.00113

168 <- 357 -0.00132

169 <- 209 -0.00119

170 <- 355 -0.00100

171 <- 203 0.00438

171 <- 212 0.00165

173 <- 218 0.00112

173 <- 234 0.00107

173 <- 242 0.00106

173 <- 265 -0.00152

173 <- 267 0.00110

175 <- 240 -0.00113

176 <- 216 0.00148

176 <- 218 -0.00449

176 <- 258 -0.00265

176 <- 267 -0.00181

176 <- 287 0.00209

177 <- 257 0.00104

177 <- 266 -0.00182

177 <- 285 0.00236

177 <- 343 -0.00100

178 <- 255 0.00192

178 <- 279 -0.00151

179 <- 254 -0.00205

179 <- 257 -0.00145

179 <- 266 -0.00161

179 <- 288 0.00129

179 <- 314 0.00174

180 <- 218 -0.00315

180 <- 275 0.00186

180 <- 287 0.00177

181 <- 255 0.00196

181 <- 282 0.00168

181 <- 284 0.00107

181 <- 292 0.00110

182 <- 210 0.00404

182 <- 339 -0.00120

183 <- 206 0.00160

183 <- 209 0.00279

183 <- 213 0.00103

183 <- 221 -0.00117

183 <- 271 0.00124

184 <- 204 0.00259

184 <- 208 0.00247

184 <- 211 0.00160

184 <- 238 -0.00178

185 <- 208 -0.00194

185 <- 211 -0.00265

185 <- 238 0.00140

185 <- 248 0.00109

185 <- 336 -0.00104

186 <- 210 -0.00205

187 <- 206 0.00311

187 <- 209 -0.00177

187 <- 213 0.00183

187 <- 221 0.00212

187 <- 241 0.00217

187 <- 245 -0.00150

187 <- 346 -0.00122

188 <- 269 0.00118

188 <- 278 -0.00157

188 <- 283 0.00105

188 <- 291 -0.00129

189 <- 230 -0.00104

189 <- 266 -0.00187

189 <- 285 0.00181

189 <- 314 0.00122

189 <- 337 -0.00141

190 <- 218 -0.00248

190 <- 265 0.00273

190 <- 271 -0.00117

190 <- 272 0.00454

190 <- 287 0.00173

190 <- 293 0.00148

190 <- 310 -0.00139

191 <- 204 -0.00143

191 <- 214 0.00104

191 <- 220 0.00167

191 <- 263 -0.00131

191 <- 269 0.00328

191 <- 278 -0.00306

191 <- 281 0.00111

191 <- 283 -0.00196

191 <- 301 0.00120

191 <- 308 -0.00156

191 <- 313 0.00203

191 <- 352 -0.00100

191 <- 417 0.00120

192 <- 204 -0.01295

192 <- 208 0.00235

192 <- 211 0.00142

192 <- 248 -0.00119

192 <- 262 -0.00184

192 <- 354 -0.00120

192 <- 364 0.00121

193 <- 205 0.00449

193 <- 210 -0.00461

193 <- 223 0.00211

193 <- 259 0.00216

193 <- 260 0.00235

194 <- 206 -0.00495

194 <- 209 0.00592

194 <- 213 0.00264

194 <- 221 0.00173

194 <- 241 0.00163

194 <- 253 0.00233

194 <- 271 0.00103

194 <- 346 0.00131

194 <- 348 0.00122

194 <- 375 0.00110

195 <- 204 -0.00268

195 <- 208 0.00671

195 <- 211 -0.00317

195 <- 238 0.00136

195 <- 248 -0.00153

195 <- 262 0.00191

195 <- 364 0.00155

196 <- 204 0.04613

196 <- 208 -0.00554

196 <- 211 0.00940

196 <- 262 -0.00205

197 <- 203 -0.00226

197 <- 264 0.00169

197 <- 273 -0.00179

197 <- 279 0.00199

197 <- 284 -0.00184

197 <- 292 0.00293

197 <- 302 -0.00100

198 <- 203 -0.01838

198 <- 207 -0.00290

198 <- 212 -0.00353

198 <- 247 0.00117

198 <- 251 0.00152

198 <- 355 0.00167

199 <- 206 -0.00199

199 <- 209 0.00279

199 <- 213 -0.00218

199 <- 221 0.00619

199 <- 241 -0.00125

199 <- 253 -0.00144

200 <- 205 0.00222

200 <- 210 0.00430

200 <- 223 -0.00172

200 <- 249 0.00245

200 <- 252 -0.00234

200 <- 259 -0.00162

200 <- 357 0.00123

200 <- 368 -0.00120

201 <- 203 -0.01270

201 <- 207 -0.00158

201 <- 212 -0.00424

201 <- 237 -0.00166

201 <- 247 0.00115

201 <- 251 -0.00273

202 <- 203 -0.07028

202 <- 212 -0.00180

202 <- 251 -0.00210

202 <- 380 -0.00179

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

132 -> 205 -0.00125

143 -> 204 -0.00123

144 -> 203 0.00123

149 -> 205 -0.00155

162 -> 206 -0.00123

164 -> 210 0.00105

167 -> 205 -0.00168

167 -> 223 0.00168

171 -> 221 -0.00214

182 -> 204 0.01016

182 -> 211 0.00123

183 -> 203 0.01016

183 -> 212 0.00123

185 -> 205 -0.00639

185 -> 223 0.00229

186 -> 204 -0.00467

187 -> 203 0.00467

192 -> 210 0.00249

192 -> 259 -0.00169

193 -> 204 -0.00827

193 -> 208 0.00143

193 -> 211 -0.00294

193 -> 262 0.00177

194 -> 203 0.00827

194 -> 207 -0.00143

194 -> 212 0.00294

194 -> 261 0.00177

195 -> 205 -0.00211

195 -> 223 0.00317

195 -> 260 0.00190

196 -> 210 0.00183

198 -> 209 0.00216

199 -> 203 -0.49935

199 -> 207 0.00318

199 -> 212 -0.00987

199 -> 237 -0.00204

199 -> 247 0.00201

200 -> 204 0.49935

200 -> 208 -0.00318

200 -> 211 0.00987

200 -> 238 -0.00204

200 -> 248 0.00201

201 -> 206 -0.01911

201 -> 221 0.01272

201 -> 245 0.00163

202 -> 209 -0.00808

202 -> 213 0.00112

149 <- 205 -0.00134

182 <- 204 0.00118

183 <- 203 0.00118

193 <- 204 0.00235

194 <- 203 -0.00235

195 <- 205 0.00233

196 <- 210 0.00145

198 <- 209 0.00179

198 <- 213 -0.00112

199 <- 203 0.00268

199 <- 207 -0.00235

199 <- 212 -0.00129

200 <- 204 -0.00268

200 <- 208 0.00235

200 <- 211 0.00129

201 <- 206 0.00328

201 <- 221 0.00109

202 <- 209 -0.00226

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

104 -> 255 0.00132

111 -> 222 -0.00114

111 -> 227 -0.00131

114 -> 224 0.00119

119 -> 230 -0.00114

119 -> 236 0.00116

120 -> 233 0.00116

123 -> 310 0.00112

123 -> 311 -0.00128

124 -> 308 0.00112

126 -> 255 0.00126

127 -> 230 -0.00119

127 -> 254 -0.00109

127 -> 257 -0.00127

129 -> 208 0.00130

131 -> 206 0.00116

133 -> 244 0.00124

134 -> 203 0.00177

136 -> 205 0.00111

138 -> 204 -0.00153

139 -> 255 0.00129

141 -> 234 0.00116

141 -> 246 -0.00132

144 -> 206 0.00171

145 -> 244 -0.00114

145 -> 330 -0.00100

147 -> 217 0.00196

147 -> 226 -0.00110

147 -> 254 -0.00109

147 -> 257 -0.00101

147 -> 270 0.00114

148 -> 215 0.00153

148 -> 225 -0.00116

149 -> 204 0.00196

149 -> 208 -0.00187

149 -> 211 -0.00139

150 -> 214 0.00141

150 -> 224 0.00111

150 -> 244 0.00111

152 -> 216 0.00231

152 -> 222 -0.00177

152 -> 242 -0.00166

152 -> 265 0.00101

153 -> 214 0.00207

153 -> 220 -0.00109

153 -> 240 0.00104

153 -> 244 0.00119

154 -> 281 -0.00105

154 -> 372 -0.00103

155 -> 235 0.00115

156 -> 216 -0.00109

156 -> 227 -0.00103

156 -> 258 0.00150

156 -> 293 0.00148

156 -> 310 0.00118

156 -> 311 -0.00107

157 -> 233 0.00105

157 -> 268 -0.00145

157 -> 341 0.00121

158 -> 293 -0.00117

159 -> 235 -0.00153

159 -> 266 -0.00185

159 -> 276 0.00124

159 -> 300 0.00102

159 -> 343 0.00145

160 -> 263 -0.00144

160 -> 308 -0.00114

161 -> 283 -0.00105

162 -> 203 -0.00202

163 -> 233 0.00104

163 -> 239 0.00113

163 -> 268 -0.00128

164 -> 204 0.00161

164 -> 208 0.00165

165 -> 205 -0.00115

166 -> 209 0.00182

166 -> 221 -0.00178

166 -> 327 0.00106

167 -> 204 0.00223

167 -> 211 0.00119

168 -> 205 0.00128

168 -> 210 0.00101

168 -> 259 -0.00159

168 -> 260 0.00149

169 -> 221 0.00168

170 -> 203 -0.00365

170 -> 207 -0.00117

170 -> 261 0.00162

171 -> 203 0.00112

171 -> 207 0.00116

171 -> 212 -0.00237

171 -> 261 -0.00121

173 -> 234 0.00115

175 -> 240 -0.00116

176 -> 218 -0.00123

178 -> 255 0.00118

178 -> 292 0.00165

179 -> 285 -0.00118

181 -> 255 0.00117

181 -> 292 0.00181

182 -> 205 -0.00568

182 -> 210 -0.00232

183 -> 206 0.00270

183 -> 209 -0.00173

183 -> 241 -0.00107

184 -> 204 -0.00292

184 -> 208 0.00315

184 -> 248 -0.00221

185 -> 204 0.00249

185 -> 208 -0.00315

185 -> 248 0.00167

186 -> 205 0.00578

186 -> 210 0.00124

186 -> 223 -0.00141

187 -> 206 0.00664

187 -> 209 -0.00397

187 -> 241 0.00104

187 -> 245 -0.00205

187 -> 253 -0.00170

187 -> 346 -0.00105

189 -> 324 -0.00101

190 -> 323 -0.00118

192 -> 204 -0.00606

192 -> 208 0.01465

192 -> 211 0.00541

192 -> 238 -0.00100

192 -> 262 0.00116

192 -> 336 0.00179

193 -> 205 0.00137

193 -> 210 0.00196

193 -> 259 -0.00114

193 -> 260 -0.00124

194 -> 206 -0.01430

194 -> 209 0.01563

194 -> 213 -0.00281

194 -> 221 -0.00613

194 -> 241 -0.00110

194 -> 253 -0.00122

194 -> 325 0.00143

194 -> 327 -0.00168

194 -> 346 0.00134

194 -> 348 0.00109

195 -> 204 -0.01708

195 -> 208 0.01391

195 -> 211 0.00720

195 -> 238 -0.00133

195 -> 248 0.00102

195 -> 336 0.00157

196 -> 204 -0.01367

196 -> 208 -0.00264

196 -> 211 -0.00220

196 -> 238 -0.00161

197 -> 203 -0.00125

197 -> 353 0.00119

198 -> 203 0.01198

198 -> 207 -0.00645

198 -> 212 0.00520

198 -> 237 0.00166

198 -> 247 -0.00133

198 -> 251 0.00148

198 -> 261 -0.00101

199 -> 206 0.01367

199 -> 221 -0.00796

199 -> 245 -0.00119

199 -> 271 -0.00101

200 -> 205 0.02397

200 -> 210 0.00195

200 -> 223 -0.00341

200 -> 249 0.00234

200 -> 252 -0.00222

200 -> 260 -0.00175

201 -> 203 0.70435

201 -> 207 -0.00372

201 -> 212 0.00832

201 -> 237 0.00118

201 -> 247 -0.00162

201 -> 251 -0.00204

201 -> 261 0.00128

202 -> 203 0.03959

202 -> 207 -0.01254

202 -> 212 0.00798

202 -> 251 -0.00298

202 -> 261 0.00103

104 <- 255 0.00101

123 <- 311 -0.00104

144 <- 206 0.00136

147 <- 217 0.00128

149 <- 204 0.00138

149 <- 208 -0.00152

149 <- 211 -0.00116

152 <- 216 0.00147

152 <- 222 -0.00113

152 <- 242 -0.00112

153 <- 214 0.00131

156 <- 258 0.00109

156 <- 293 0.00112

157 <- 268 -0.00105

159 <- 266 -0.00132

159 <- 343 0.00115

160 <- 263 -0.00106

162 <- 203 -0.00132

164 <- 208 0.00120

166 <- 209 0.00136

167 <- 204 0.00155

168 <- 205 0.00186

168 <- 210 0.00113

168 <- 259 -0.00128

168 <- 260 0.00118

170 <- 203 -0.00230

170 <- 207 -0.00146

170 <- 261 0.00127

171 <- 203 0.00358

171 <- 212 -0.00120

171 <- 261 -0.00103

178 <- 292 0.00121

181 <- 292 0.00132

182 <- 205 -0.00330

182 <- 210 -0.00140

183 <- 206 0.00225

183 <- 209 -0.00215

185 <- 204 0.00118

185 <- 208 -0.00126

187 <- 206 0.00174

187 <- 209 -0.00167

187 <- 245 -0.00108

192 <- 204 -0.00133

192 <- 208 0.00796

192 <- 211 0.00321

192 <- 336 0.00122

193 <- 205 -0.00146

194 <- 206 -0.00744

194 <- 209 0.00787

194 <- 213 -0.00155

194 <- 221 -0.00316

194 <- 327 -0.00113

195 <- 204 -0.00366

195 <- 208 0.00671

195 <- 211 0.00398

195 <- 336 0.00105

196 <- 208 -0.00203

196 <- 211 -0.00166

196 <- 238 -0.00104

198 <- 203 0.00455

198 <- 212 0.00128

198 <- 251 0.00115

198 <- 261 -0.00104

199 <- 206 -0.00218

200 <- 205 -0.00842

200 <- 210 -0.00354

200 <- 249 0.00169

200 <- 252 -0.00161

200 <- 259 0.00204

200 <- 260 -0.00145

201 <- 203 -0.01431

201 <- 207 -0.00129

201 <- 212 0.00299

201 <- 247 -0.00101

201 <- 251 -0.00153

201 <- 261 0.00174

202 <- 203 -0.01787

202 <- 207 -0.00724

202 <- 212 0.00672

202 <- 237 0.00102

202 <- 251 -0.00128

202 <- 261 0.00146

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

104 -> 256 -0.00132

110 -> 222 0.00114

110 -> 227 -0.00131

114 -> 225 -0.00119

118 -> 230 -0.00114

118 -> 236 -0.00116

120 -> 232 -0.00116

122 -> 310 -0.00112

122 -> 311 -0.00128

124 -> 309 -0.00112

126 -> 256 0.00126

128 -> 230 -0.00119

128 -> 254 -0.00109

128 -> 257 0.00127

129 -> 207 0.00130

130 -> 206 -0.00116

133 -> 243 0.00124

134 -> 204 0.00177

135 -> 205 0.00111

138 -> 203 -0.00153

139 -> 256 -0.00129

140 -> 234 0.00116

140 -> 246 0.00132

143 -> 206 -0.00171

145 -> 243 0.00114

145 -> 331 0.00100

146 -> 217 0.00196

146 -> 226 0.00110

146 -> 254 -0.00109

146 -> 257 0.00101

146 -> 270 -0.00114

148 -> 214 -0.00153

148 -> 224 0.00116

149 -> 203 -0.00196

149 -> 207 0.00187

149 -> 212 0.00139

150 -> 215 0.00141

150 -> 225 0.00111

150 -> 243 0.00111

151 -> 216 0.00231

151 -> 222 0.00177

151 -> 242 -0.00166

151 -> 265 -0.00101

153 -> 215 -0.00207

153 -> 219 0.00109

153 -> 239 -0.00104

153 -> 243 -0.00119

154 -> 282 -0.00105

154 -> 371 -0.00103

155 -> 216 0.00109

155 -> 227 0.00103

155 -> 258 -0.00150

155 -> 293 0.00148

155 -> 310 0.00118

155 -> 311 0.00107

156 -> 235 -0.00115

157 -> 232 0.00105

157 -> 269 -0.00145

157 -> 340 0.00121

158 -> 235 -0.00153

158 -> 266 -0.00185

158 -> 276 -0.00124

158 -> 300 -0.00102

158 -> 343 0.00145

159 -> 293 0.00117

160 -> 264 0.00144

160 -> 309 0.00114

161 -> 284 -0.00105

162 -> 204 -0.00202

163 -> 232 -0.00104

163 -> 240 -0.00113

163 -> 269 0.00128

164 -> 203 0.00161

164 -> 207 0.00165

165 -> 209 0.00182

165 -> 221 0.00178

165 -> 327 0.00106

166 -> 205 -0.00115

167 -> 203 -0.00223

167 -> 212 -0.00119

168 -> 221 -0.00168

169 -> 205 0.00128

169 -> 210 -0.00101

169 -> 259 0.00159

169 -> 260 0.00149

170 -> 204 0.00365

170 -> 208 0.00117

170 -> 262 0.00162

171 -> 204 0.00112

171 -> 208 0.00116

171 -> 211 -0.00237

171 -> 262 0.00121

174 -> 234 0.00115

175 -> 239 0.00116

177 -> 218 -0.00123

178 -> 256 0.00118

178 -> 291 0.00165

180 -> 285 -0.00118

181 -> 256 -0.00117

181 -> 291 -0.00181

182 -> 206 0.00270

182 -> 209 0.00173

182 -> 241 0.00107

183 -> 205 0.00568

183 -> 210 -0.00232

184 -> 203 -0.00292

184 -> 207 0.00315

184 -> 247 0.00221

185 -> 203 -0.00249

185 -> 207 0.00315

185 -> 247 0.00167

186 -> 206 -0.00664

186 -> 209 -0.00397

186 -> 241 0.00104

186 -> 245 0.00205

186 -> 253 -0.00170

186 -> 346 0.00105

187 -> 205 0.00578

187 -> 210 -0.00124

187 -> 223 -0.00141

189 -> 323 -0.00118

190 -> 324 0.00101

192 -> 203 -0.00606

192 -> 207 0.01465

192 -> 212 0.00541

192 -> 237 0.00100

192 -> 261 -0.00116

192 -> 335 0.00179

193 -> 206 0.01430

193 -> 209 0.01563

193 -> 213 -0.00281

193 -> 221 0.00613

193 -> 241 -0.00110

193 -> 253 -0.00122

193 -> 325 -0.00143

193 -> 327 -0.00168

193 -> 346 -0.00134

193 -> 348 0.00109

194 -> 205 0.00137

194 -> 210 -0.00196

194 -> 259 0.00114

194 -> 260 -0.00124

195 -> 203 0.01708

195 -> 207 -0.01391

195 -> 212 -0.00720

195 -> 237 -0.00133

195 -> 247 0.00102

195 -> 335 -0.00157

196 -> 203 -0.01367

196 -> 207 -0.00264

196 -> 212 -0.00220

196 -> 237 0.00161

197 -> 204 0.00125

197 -> 352 0.00119

198 -> 204 -0.01198

198 -> 208 0.00645

198 -> 211 -0.00520

198 -> 238 0.00166

198 -> 248 -0.00133

198 -> 250 -0.00148

198 -> 262 -0.00101

199 -> 205 0.02397

199 -> 210 -0.00195

199 -> 223 -0.00341

199 -> 249 0.00234

199 -> 252 0.00222

199 -> 260 -0.00175

200 -> 206 -0.01367

200 -> 221 0.00796

200 -> 245 0.00119

200 -> 271 -0.00101

201 -> 204 0.70435

201 -> 208 -0.00372

201 -> 211 0.00832

201 -> 238 -0.00118

201 -> 248 0.00162

201 -> 250 -0.00204

201 -> 262 -0.00128

202 -> 204 -0.03959

202 -> 208 0.01254

202 -> 211 -0.00798

202 -> 250 0.00298

202 -> 262 0.00103

104 <- 256 -0.00101

122 <- 311 -0.00104

143 <- 206 -0.00136

146 <- 217 0.00128

149 <- 203 -0.00138

149 <- 207 0.00152

149 <- 212 0.00116

151 <- 216 0.00147

151 <- 222 0.00113

151 <- 242 -0.00112

153 <- 215 -0.00131

155 <- 258 -0.00109

155 <- 293 0.00112

157 <- 269 -0.00105

158 <- 266 -0.00132

158 <- 343 0.00115

160 <- 264 0.00106

162 <- 204 -0.00132

164 <- 207 0.00120

165 <- 209 0.00136

167 <- 203 -0.00155

169 <- 205 0.00186

169 <- 210 -0.00113

169 <- 259 0.00128

169 <- 260 0.00118

170 <- 204 0.00230

170 <- 208 0.00146

170 <- 262 0.00127

171 <- 204 0.00358

171 <- 211 -0.00120

171 <- 262 0.00103

178 <- 291 0.00121

181 <- 291 -0.00132

182 <- 206 0.00225

182 <- 209 0.00215

183 <- 205 0.00330

183 <- 210 -0.00140

185 <- 203 -0.00118

185 <- 207 0.00126

186 <- 206 -0.00174

186 <- 209 -0.00167

186 <- 245 0.00108

192 <- 203 -0.00133

192 <- 207 0.00796

192 <- 212 0.00321

192 <- 335 0.00122

193 <- 206 0.00744

193 <- 209 0.00787

193 <- 213 -0.00155

193 <- 221 0.00316

193 <- 327 -0.00113

194 <- 205 -0.00146

195 <- 203 0.00366

195 <- 207 -0.00671

195 <- 212 -0.00398

195 <- 335 -0.00105

196 <- 207 -0.00203

196 <- 212 -0.00166

196 <- 237 0.00104

198 <- 204 -0.00455

198 <- 211 -0.00128

198 <- 250 -0.00115

198 <- 262 -0.00104

199 <- 205 -0.00842

199 <- 210 0.00354

199 <- 249 0.00169

199 <- 252 0.00161

199 <- 259 -0.00204

199 <- 260 -0.00145

200 <- 206 0.00218

201 <- 204 -0.01431

201 <- 208 -0.00129

201 <- 211 0.00299

201 <- 248 0.00101

201 <- 250 -0.00153

201 <- 262 -0.00174

202 <- 204 0.01787

202 <- 208 0.00724

202 <- 211 -0.00672

202 <- 238 0.00102

202 <- 250 0.00128

202 <- 262 0.00146

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

69 -> 258 0.00111

125 -> 272 -0.00194

129 -> 223 0.00104

138 -> 205 -0.00241

138 -> 223 0.00180

143 -> 204 -0.00262

143 -> 238 -0.00107

144 -> 203 -0.00262

144 -> 237 0.00107

154 -> 289 -0.00101

162 -> 209 0.00183

162 -> 241 0.00132

162 -> 253 0.00143

164 -> 205 0.00183

165 -> 204 -0.00435

166 -> 203 -0.00435

168 -> 204 -0.00421

168 -> 211 -0.00161

169 -> 203 -0.00421

169 -> 212 -0.00161

170 -> 221 0.00238

171 -> 241 -0.00159

182 -> 204 -0.01025

182 -> 211 -0.00164

182 -> 238 -0.00121

183 -> 203 0.01025

183 -> 212 0.00164

183 -> 237 -0.00121

184 -> 205 0.00384

184 -> 223 -0.00128

185 -> 210 0.00107

186 -> 204 0.00388

186 -> 211 0.00117

187 -> 203 0.00388

187 -> 212 0.00117

188 -> 230 0.00171

188 -> 266 0.00101

188 -> 407 -0.00120

189 -> 204 0.00150

189 -> 274 0.00104

189 -> 278 -0.00165

189 -> 281 0.00105

189 -> 291 -0.00149

189 -> 299 -0.00147

189 -> 352 0.00112

190 -> 203 -0.00150

190 -> 273 0.00104

190 -> 279 -0.00165

190 -> 282 0.00105

190 -> 292 -0.00149

190 -> 298 -0.00147

190 -> 353 0.00112

192 -> 205 0.00819

192 -> 260 0.00143

193 -> 204 -0.01680

193 -> 208 -0.00169

193 -> 211 0.00208

193 -> 262 -0.00180

194 -> 203 -0.01680

194 -> 207 -0.00169

194 -> 212 0.00208

194 -> 261 0.00180

195 -> 210 0.00340

195 -> 259 -0.00184

196 -> 205 -0.00580

196 -> 223 0.00514

196 -> 260 0.00195

196 -> 339 0.00112

197 -> 206 0.00138

197 -> 221 -0.00101

197 -> 267 -0.00155

197 -> 287 -0.00233

197 -> 290 0.00196

197 -> 323 -0.00197

197 -> 347 -0.00133

197 -> 367 -0.00176

197 -> 386 0.00107

198 -> 206 0.01700

198 -> 221 -0.01262

198 -> 245 -0.00159

199 -> 203 0.49916

199 -> 207 -0.00246

199 -> 212 0.00897

199 -> 237 0.00388

199 -> 239 0.00189

199 -> 247 -0.00309

200 -> 204 0.49916

200 -> 208 -0.00246

200 -> 211 0.00897

200 -> 238 -0.00388

200 -> 240 -0.00189

200 -> 248 0.00309

201 -> 209 -0.00532

201 -> 213 0.00101

201 -> 241 0.00166

201 -> 253 0.00205

201 -> 271 -0.00155

202 -> 206 0.00410

202 -> 221 0.00271

125 <- 272 -0.00150

138 <- 205 -0.00119

138 <- 223 0.00129

143 <- 204 -0.00134

144 <- 203 -0.00134

162 <- 209 0.00186

162 <- 241 0.00112

162 <- 253 0.00112

164 <- 205 0.00109

165 <- 204 -0.00185

166 <- 203 -0.00185

168 <- 204 -0.00126

169 <- 203 -0.00126

182 <- 204 -0.00599

182 <- 211 -0.00184

183 <- 203 0.00599

183 <- 212 0.00184

186 <- 204 0.00226

186 <- 211 0.00113

187 <- 203 0.00226

187 <- 212 0.00113

189 <- 278 -0.00113

189 <- 291 -0.00103

189 <- 299 -0.00104

190 <- 279 -0.00113

190 <- 292 -0.00103

190 <- 298 -0.00104

192 <- 205 0.00310

193 <- 204 -0.00153

193 <- 211 0.00167

193 <- 262 -0.00119

194 <- 203 -0.00153

194 <- 212 0.00167

194 <- 261 0.00119

195 <- 210 0.00199

195 <- 259 -0.00107

196 <- 205 -0.00398

196 <- 223 0.00469

196 <- 260 0.00175

197 <- 287 -0.00160

197 <- 290 0.00134

197 <- 323 -0.00143

197 <- 367 -0.00134

198 <- 221 -0.00394

199 <- 203 -0.00201

199 <- 207 0.00246

199 <- 237 0.00136

199 <- 247 -0.00119

200 <- 204 -0.00201

200 <- 208 0.00246

200 <- 238 -0.00136

200 <- 248 0.00119

201 <- 209 -0.00309

201 <- 213 0.00102

201 <- 253 0.00126

202 <- 206 0.00603

202 <- 221 -0.00306

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

96 -> 227 -0.00101

97 -> 300 0.00122

98 -> 222 0.00100

98 -> 231 0.00103

98 -> 286 -0.00114

98 -> 293 0.00126

99 -> 292 -0.00102

100 -> 291 -0.00102

101 -> 242 -0.00102

101 -> 290 -0.00111

102 -> 243 -0.00107

102 -> 255 0.00129

102 -> 312 0.00111

103 -> 244 -0.00107

103 -> 256 0.00129

103 -> 313 0.00111

104 -> 254 0.00177

104 -> 266 0.00146

104 -> 280 -0.00110

104 -> 343 -0.00125

110 -> 225 0.00127

111 -> 224 -0.00127

113 -> 222 -0.00141

113 -> 246 0.00111

114 -> 227 0.00191

117 -> 236 0.00143

117 -> 257 0.00103

118 -> 232 0.00145

119 -> 233 -0.00145

120 -> 230 0.00169

121 -> 246 -0.00104

121 -> 277 -0.00104

121 -> 286 0.00108

121 -> 293 -0.00114

121 -> 310 -0.00141

122 -> 284 0.00117

122 -> 309 0.00120

123 -> 283 -0.00117

123 -> 308 -0.00120

124 -> 267 -0.00115

124 -> 290 -0.00132

124 -> 311 0.00172

126 -> 257 0.00152

126 -> 270 0.00104

127 -> 229 0.00121

127 -> 255 -0.00137

128 -> 228 -0.00121

128 -> 256 0.00137

129 -> 206 0.00229

130 -> 207 -0.00135

131 -> 208 0.00135

132 -> 209 0.00112

133 -> 246 0.00158

133 -> 286 0.00109

133 -> 338 0.00108

134 -> 210 0.00101

135 -> 204 -0.00180

136 -> 203 0.00180

137 -> 205 -0.00156

138 -> 206 0.00273

139 -> 230 0.00125

139 -> 254 0.00150

140 -> 243 0.00142

140 -> 284 0.00108

141 -> 244 -0.00142

141 -> 283 -0.00108

142 -> 226 -0.00141

142 -> 257 -0.00115

142 -> 270 0.00138

143 -> 203 0.00198

143 -> 207 -0.00257

144 -> 204 -0.00198

144 -> 208 0.00257

145 -> 234 0.00183

145 -> 329 0.00151

146 -> 214 0.00129

146 -> 224 -0.00168

146 -> 256 0.00128

147 -> 215 -0.00129

147 -> 225 0.00168

147 -> 255 -0.00128

148 -> 217 -0.00286

148 -> 254 0.00127

148 -> 266 -0.00128

149 -> 209 0.00294

149 -> 213 -0.00181

150 -> 222 0.00225

150 -> 231 0.00118

150 -> 246 0.00101

150 -> 265 -0.00131

151 -> 215 0.00240

151 -> 219 -0.00124

151 -> 243 0.00143

152 -> 214 -0.00240

152 -> 220 0.00124

152 -> 244 -0.00143

153 -> 216 -0.00328

153 -> 218 -0.00100

153 -> 234 0.00101

153 -> 242 0.00219

153 -> 332 -0.00115

154 -> 277 0.00111

154 -> 293 -0.00190

154 -> 310 -0.00160

154 -> 365 -0.00133

155 -> 215 0.00115

155 -> 229 0.00102

155 -> 268 -0.00129

155 -> 309 -0.00158

155 -> 331 -0.00104

155 -> 371 0.00105

156 -> 214 0.00115

156 -> 228 0.00102

156 -> 269 -0.00129

156 -> 308 -0.00158

156 -> 330 -0.00104

156 -> 372 0.00105

157 -> 236 -0.00135

157 -> 270 0.00117

157 -> 276 -0.00197

157 -> 300 -0.00121

157 -> 337 0.00125

158 -> 240 0.00115

158 -> 263 0.00131

158 -> 269 -0.00125

158 -> 274 -0.00106

158 -> 283 0.00104

158 -> 340 0.00129

159 -> 239 -0.00115

159 -> 264 -0.00131

159 -> 268 0.00125

159 -> 273 0.00106

159 -> 284 -0.00104

159 -> 341 -0.00129

160 -> 216 -0.00105

160 -> 227 -0.00137

160 -> 258 0.00180

160 -> 267 -0.00122

160 -> 290 0.00107

160 -> 311 -0.00152

160 -> 332 0.00122

160 -> 386 0.00138

163 -> 235 0.00231

163 -> 266 0.00212

163 -> 343 -0.00203

164 -> 221 0.00361

164 -> 325 0.00105

165 -> 203 0.00193

165 -> 212 0.00184

165 -> 237 0.00160

165 -> 247 -0.00141

166 -> 204 -0.00193

166 -> 211 -0.00184

166 -> 238 0.00160

166 -> 248 -0.00141

167 -> 253 0.00111

167 -> 271 -0.00135

167 -> 327 -0.00134

168 -> 207 0.00143

168 -> 212 -0.00150

168 -> 261 -0.00194

169 -> 208 -0.00143

169 -> 211 0.00150

169 -> 262 -0.00194

170 -> 205 -0.00198

170 -> 223 -0.00141

170 -> 260 -0.00221

171 -> 210 0.00314

171 -> 259 -0.00195

171 -> 357 -0.00128

172 -> 222 -0.00120

172 -> 265 -0.00139

172 -> 310 -0.00118

173 -> 240 0.00109

173 -> 263 0.00126

174 -> 239 -0.00109

174 -> 264 -0.00126

175 -> 234 -0.00160

175 -> 242 -0.00123

175 -> 275 -0.00119

175 -> 323 0.00111

176 -> 269 -0.00105

176 -> 281 -0.00112

176 -> 291 -0.00120

177 -> 268 0.00105

177 -> 282 0.00112

177 -> 292 0.00120

178 -> 236 0.00105

178 -> 257 0.00140

178 -> 270 -0.00138

178 -> 288 -0.00159

178 -> 300 0.00132

179 -> 229 -0.00111

179 -> 255 -0.00125

179 -> 292 -0.00163

180 -> 228 0.00111

180 -> 256 0.00125

180 -> 291 0.00163

181 -> 230 -0.00142

181 -> 254 0.00153

181 -> 266 -0.00118

181 -> 285 0.00176

181 -> 303 0.00103

182 -> 203 -0.00210

182 -> 212 0.00365

182 -> 247 -0.00108

183 -> 204 -0.00210

183 -> 211 0.00365

183 -> 248 0.00108

184 -> 206 0.00641

184 -> 221 -0.00158

184 -> 245 -0.00266

185 -> 209 0.00455

185 -> 213 -0.00118

185 -> 241 -0.00124

185 -> 253 0.00230

185 -> 348 0.00112

186 -> 203 0.00433

186 -> 207 -0.00466

186 -> 212 -0.00231

186 -> 247 -0.00244

187 -> 204 -0.00433

187 -> 208 0.00466

187 -> 211 0.00231

187 -> 248 -0.00244

188 -> 265 0.00120

188 -> 272 0.00211

189 -> 279 0.00122

190 -> 278 -0.00122

191 -> 216 -0.00204

191 -> 218 0.00557

191 -> 258 0.00221

191 -> 267 0.00136

191 -> 287 -0.00131

191 -> 420 -0.00106

191 -> 428 0.00109

192 -> 206 0.01569

192 -> 221 0.00936

192 -> 325 -0.00213

192 -> 346 -0.00172

193 -> 203 -0.01284

193 -> 207 0.01616

193 -> 212 0.00713

193 -> 237 0.00304

193 -> 239 0.00151

193 -> 247 -0.00201

193 -> 318 -0.00146

193 -> 335 0.00184

194 -> 204 0.01284

194 -> 208 -0.01616

194 -> 211 -0.00713

194 -> 238 0.00304

194 -> 240 0.00151

194 -> 248 -0.00201

194 -> 319 0.00146

194 -> 336 -0.00184

195 -> 209 -0.01880

195 -> 213 0.00302

195 -> 241 0.00263

195 -> 253 0.00282

195 -> 271 -0.00145

195 -> 327 0.00229

195 -> 348 -0.00123

196 -> 206 0.00100

196 -> 221 -0.00319

197 -> 205 -0.00371

197 -> 288 0.00114

197 -> 324 -0.00195

198 -> 205 -0.03688

198 -> 223 0.00497

198 -> 249 -0.00165

198 -> 260 0.00242

199 -> 204 -0.49780

199 -> 211 -0.00656

199 -> 250 0.00289

199 -> 262 0.00249

200 -> 203 0.49780

200 -> 212 0.00656

200 -> 251 -0.00289

200 -> 261 0.00249

201 -> 252 -0.00293

201 -> 259 0.00149

202 -> 205 -0.04246

202 -> 223 -0.00661

202 -> 249 0.00365

202 -> 368 -0.00105

97 <- 300 0.00102

98 <- 293 0.00103

104 <- 254 0.00135

104 <- 266 0.00115

104 <- 343 -0.00110

114 <- 227 0.00136

117 <- 236 0.00101

118 <- 232 0.00102

119 <- 233 -0.00102

120 <- 230 0.00118

121 <- 310 -0.00114

124 <- 290 -0.00102

124 <- 311 0.00139

126 <- 257 0.00112

127 <- 255 -0.00101

128 <- 256 0.00101

129 <- 206 0.00135

133 <- 246 0.00112

137 <- 205 -0.00109

138 <- 206 0.00209

139 <- 254 0.00108

143 <- 203 0.00125

143 <- 207 -0.00207

144 <- 204 -0.00125

144 <- 208 0.00207

145 <- 234 0.00126

145 <- 329 0.00117

146 <- 224 -0.00111

147 <- 225 0.00111

148 <- 217 -0.00186

149 <- 209 0.00263

149 <- 213 -0.00134

150 <- 222 0.00144

151 <- 215 0.00152

152 <- 214 -0.00152

153 <- 216 -0.00207

153 <- 242 0.00146

154 <- 293 -0.00145

154 <- 310 -0.00125

154 <- 365 -0.00103

155 <- 309 -0.00122

156 <- 308 -0.00122

157 <- 276 -0.00142

158 <- 340 0.00102

159 <- 341 -0.00102

160 <- 258 0.00131

160 <- 311 -0.00118

160 <- 386 0.00109

163 <- 235 0.00149

163 <- 266 0.00151

163 <- 343 -0.00160

164 <- 221 0.00201

165 <- 203 0.00104

165 <- 212 0.00104

166 <- 204 -0.00104

166 <- 211 -0.00104

168 <- 203 0.00193

168 <- 207 0.00166

168 <- 212 -0.00116

168 <- 261 -0.00156

169 <- 204 -0.00193

169 <- 208 -0.00166

169 <- 211 0.00116

169 <- 262 -0.00156

170 <- 205 -0.00293

170 <- 260 -0.00173

171 <- 210 0.00231

171 <- 259 -0.00160

178 <- 288 -0.00115

179 <- 292 -0.00120

180 <- 291 0.00120

181 <- 285 0.00124

182 <- 203 -0.00297

182 <- 207 0.00147

182 <- 212 0.00188

183 <- 204 -0.00297

183 <- 208 0.00147

183 <- 211 0.00188

184 <- 245 -0.00140

185 <- 209 0.00137

186 <- 203 0.00218

186 <- 207 -0.00174

186 <- 247 -0.00117

187 <- 204 -0.00218

187 <- 208 0.00174

187 <- 248 -0.00117

188 <- 272 0.00140

191 <- 216 -0.00101

191 <- 218 0.00274

191 <- 258 0.00130

192 <- 206 0.00857

192 <- 221 0.00531

192 <- 325 -0.00143

192 <- 346 -0.00121

193 <- 203 -0.00183

193 <- 207 0.00775

193 <- 212 0.00446

193 <- 237 0.00173

193 <- 247 -0.00134

193 <- 335 0.00127

194 <- 204 0.00183

194 <- 208 -0.00775

194 <- 211 -0.00446

194 <- 238 0.00173

194 <- 248 -0.00134

194 <- 336 -0.00127

195 <- 209 -0.00944

195 <- 213 0.00177

195 <- 241 0.00134

195 <- 253 0.00167

195 <- 327 0.00154

196 <- 206 -0.00348

197 <- 324 -0.00139

198 <- 205 0.00151

198 <- 249 -0.00148

198 <- 260 0.00190

199 <- 204 0.01364

199 <- 208 0.00264

199 <- 211 -0.00349

199 <- 250 0.00197

199 <- 262 0.00259

200 <- 203 -0.01364

200 <- 207 -0.00264

200 <- 212 0.00349

200 <- 251 -0.00197

200 <- 261 0.00259

201 <- 210 -0.00552

201 <- 252 -0.00213

201 <- 259 0.00295

202 <- 205 -0.02169

202 <- 223 -0.00218

202 <- 249 0.00160

202 <- 260 -0.00124

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

69 -> 280 0.00111

72 -> 258 0.00111

96 -> 286 0.00110

96 -> 293 -0.00113

97 -> 266 -0.00106

98 -> 275 -0.00101

98 -> 290 0.00148

98 -> 311 -0.00116

99 -> 284 0.00155

100 -> 283 -0.00155

102 -> 255 0.00100

102 -> 292 -0.00107

103 -> 256 -0.00100

103 -> 291 0.00107

104 -> 257 0.00136

104 -> 270 0.00144

104 -> 300 -0.00167

113 -> 227 -0.00118

114 -> 222 0.00109

117 -> 254 0.00103

117 -> 266 0.00107

117 -> 314 0.00107

118 -> 301 0.00106

119 -> 302 -0.00106

121 -> 218 -0.00132

121 -> 258 -0.00136

121 -> 267 -0.00104

121 -> 290 -0.00164

121 -> 311 0.00179

122 -> 282 0.00131

122 -> 284 -0.00194

122 -> 309 -0.00137

122 -> 331 -0.00102

123 -> 281 0.00131

123 -> 283 -0.00194

123 -> 308 -0.00137

123 -> 330 -0.00102

124 -> 277 -0.00128

124 -> 286 0.00184

124 -> 293 -0.00169

124 -> 310 -0.00172

126 -> 230 0.00182

126 -> 254 0.00165

126 -> 266 0.00177

126 -> 289 -0.00168

126 -> 326 0.00135

126 -> 343 -0.00139

127 -> 229 0.00116

127 -> 255 -0.00153

127 -> 264 -0.00173

127 -> 279 0.00135

127 -> 312 -0.00124

128 -> 228 0.00116

128 -> 256 -0.00153

128 -> 263 -0.00173

128 -> 278 0.00135

128 -> 313 -0.00124

129 -> 209 -0.00131

130 -> 207 0.00108

131 -> 208 0.00108

132 -> 206 -0.00129

133 -> 218 -0.00125

133 -> 234 -0.00212

133 -> 258 0.00111

133 -> 267 -0.00203

133 -> 275 0.00135

134 -> 205 0.00187

135 -> 204 0.00197

135 -> 211 -0.00101

136 -> 203 0.00197

136 -> 212 -0.00101

137 -> 210 -0.00134

138 -> 209 -0.00127

138 -> 213 -0.00155

138 -> 348 0.00102

139 -> 257 0.00141

139 -> 270 0.00104

139 -> 300 -0.00111

140 -> 239 0.00118

140 -> 268 0.00103

140 -> 273 -0.00113

140 -> 284 -0.00127

140 -> 317 -0.00106

140 -> 331 -0.00105

141 -> 240 0.00118

141 -> 269 0.00103

141 -> 274 -0.00113

141 -> 283 -0.00127

141 -> 316 0.00106

141 -> 330 -0.00105

143 -> 203 -0.00372

143 -> 207 0.00121

143 -> 318 -0.00161

144 -> 204 -0.00372

144 -> 208 0.00121

144 -> 319 -0.00161

145 -> 231 0.00105

145 -> 246 -0.00115

145 -> 265 -0.00118

145 -> 277 0.00154

145 -> 286 -0.00204

145 -> 310 0.00136

145 -> 338 -0.00158

148 -> 270 -0.00109

149 -> 206 -0.00375

150 -> 216 -0.00144

151 -> 264 -0.00110

152 -> 263 -0.00110

153 -> 222 0.00137

154 -> 227 0.00157

154 -> 234 0.00282

154 -> 242 -0.00151

154 -> 258 -0.00297

154 -> 267 0.00187

154 -> 275 -0.00112

154 -> 290 -0.00209

154 -> 311 0.00178

154 -> 332 -0.00162

154 -> 386 -0.00129

155 -> 239 0.00159

155 -> 243 -0.00197

155 -> 264 0.00269

155 -> 273 -0.00168

155 -> 282 -0.00190

155 -> 284 0.00147

155 -> 309 0.00125

155 -> 312 0.00162

155 -> 331 0.00128

155 -> 341 0.00113

155 -> 371 -0.00113

156 -> 240 -0.00159

156 -> 244 0.00197

156 -> 263 -0.00269

156 -> 274 0.00168

156 -> 281 0.00190

156 -> 283 -0.00147

156 -> 308 -0.00125

156 -> 313 -0.00162

156 -> 330 -0.00128

156 -> 340 -0.00113

156 -> 372 0.00113

157 -> 230 0.00162

157 -> 235 0.00126

157 -> 254 0.00119

157 -> 266 0.00338

157 -> 280 -0.00112

157 -> 289 -0.00176

157 -> 343 -0.00241

158 -> 232 -0.00168

158 -> 244 -0.00133

158 -> 256 -0.00112

158 -> 269 0.00301

158 -> 278 0.00105

158 -> 281 -0.00118

158 -> 291 0.00172

158 -> 301 0.00194

158 -> 308 0.00169

158 -> 316 0.00120

159 -> 233 -0.00168

159 -> 243 -0.00133

159 -> 255 -0.00112

159 -> 268 0.00301

159 -> 279 0.00105

159 -> 282 -0.00118

159 -> 292 0.00172

159 -> 302 -0.00194

159 -> 309 0.00169

159 -> 317 -0.00120

160 -> 231 -0.00151

160 -> 246 0.00296

160 -> 265 0.00217

160 -> 277 -0.00164

160 -> 293 0.00434

160 -> 310 0.00192

160 -> 320 -0.00102

160 -> 328 0.00141

160 -> 365 0.00127

161 -> 227 0.00218

161 -> 234 0.00113

161 -> 267 0.00166

161 -> 275 -0.00175

161 -> 290 0.00275

161 -> 311 -0.00204

161 -> 329 0.00100

162 -> 205 -0.00482

162 -> 339 0.00198

163 -> 205 -0.00120

163 -> 236 -0.00158

163 -> 257 0.00130

163 -> 270 0.00254

163 -> 276 -0.00196

163 -> 300 -0.00244

163 -> 315 0.00147

163 -> 337 0.00181

164 -> 209 -0.00283

164 -> 213 0.00222

165 -> 203 -0.00202

165 -> 207 -0.00308

165 -> 212 -0.00146

165 -> 318 -0.00107

166 -> 204 -0.00202

166 -> 208 -0.00308

166 -> 211 -0.00146

166 -> 319 -0.00107

167 -> 221 0.00213

167 -> 325 0.00133

168 -> 203 0.00470

168 -> 207 0.00126

168 -> 212 -0.00227

168 -> 261 -0.00172

169 -> 204 0.00470

169 -> 208 0.00126

169 -> 211 -0.00227

169 -> 262 0.00172

170 -> 210 -0.00343

170 -> 259 0.00173

171 -> 205 0.00944

171 -> 223 0.00183

171 -> 260 0.00195

171 -> 339 -0.00161

176 -> 220 0.00155

176 -> 224 -0.00134

176 -> 228 0.00165

176 -> 274 0.00135

176 -> 278 0.00125

176 -> 283 0.00175

176 -> 291 0.00149

176 -> 308 0.00115

177 -> 219 0.00155

177 -> 225 -0.00134

177 -> 229 0.00165

177 -> 273 0.00135

177 -> 279 0.00125

177 -> 284 0.00175

177 -> 292 0.00149

177 -> 309 0.00115

178 -> 230 -0.00113

178 -> 266 -0.00179

178 -> 280 0.00141

178 -> 289 0.00104

178 -> 343 0.00123

179 -> 219 0.00110

179 -> 225 -0.00133

179 -> 268 -0.00167

179 -> 273 0.00123

179 -> 284 0.00197

179 -> 292 -0.00152

179 -> 317 0.00107

179 -> 353 -0.00113

180 -> 220 0.00110

180 -> 224 -0.00133

180 -> 269 -0.00167

180 -> 274 0.00123

180 -> 283 0.00197

180 -> 291 -0.00152

180 -> 316 -0.00107

180 -> 352 -0.00113

181 -> 270 -0.00192

181 -> 300 0.00230

181 -> 337 -0.00179

182 -> 203 -0.00335

182 -> 207 -0.00891

182 -> 212 0.00362

182 -> 237 0.00161

182 -> 335 -0.00116

182 -> 355 -0.00151

183 -> 204 0.00335

183 -> 208 0.00891

183 -> 211 -0.00362

183 -> 238 0.00161

183 -> 336 0.00116

183 -> 354 0.00151

184 -> 209 0.00165

184 -> 253 -0.00115

185 -> 206 -0.00410

185 -> 221 0.00167

185 -> 245 0.00149

186 -> 203 -0.00139

186 -> 207 0.00407

186 -> 212 -0.00141

186 -> 247 0.00170

187 -> 204 -0.00139

187 -> 208 0.00407

187 -> 211 -0.00141

187 -> 248 -0.00170

188 -> 216 0.00148

188 -> 242 -0.00161

188 -> 258 0.00199

188 -> 267 -0.00129

188 -> 275 0.00149

188 -> 287 0.00149

188 -> 323 -0.00237

188 -> 329 -0.00101

188 -> 347 -0.00153

188 -> 351 -0.00195

188 -> 367 -0.00126

188 -> 411 -0.00120

188 -> 440 -0.00210

189 -> 215 -0.00214

189 -> 233 0.00170

189 -> 255 -0.00102

189 -> 264 -0.00188

189 -> 273 0.00124

189 -> 282 0.00136

189 -> 292 0.00140

189 -> 298 -0.00169

189 -> 317 0.00137

189 -> 331 0.00108

189 -> 333 -0.00118

189 -> 353 0.00157

189 -> 362 0.00154

189 -> 382 0.00100

189 -> 390 0.00103

189 -> 403 0.00110

189 -> 427 0.00103

189 -> 437 -0.00101

189 -> 447 0.00128

190 -> 214 -0.00214

190 -> 232 0.00170

190 -> 256 -0.00102

190 -> 263 -0.00188

190 -> 274 0.00124

190 -> 281 0.00136

190 -> 291 0.00140

190 -> 299 -0.00169

190 -> 316 -0.00137

190 -> 330 0.00108

190 -> 334 0.00118

190 -> 352 0.00157

190 -> 361 0.00154

190 -> 383 0.00100

190 -> 391 0.00103

190 -> 404 -0.00110

190 -> 426 -0.00103

190 -> 436 -0.00101

190 -> 448 0.00128

191 -> 222 0.00279

191 -> 231 0.00279

191 -> 246 -0.00126

191 -> 277 0.00241

191 -> 286 -0.00298

191 -> 310 0.00128

191 -> 338 -0.00140

192 -> 209 -0.03196

192 -> 213 0.00759

192 -> 241 -0.00103

192 -> 271 0.00176

192 -> 327 0.00245

192 -> 348 -0.00120

193 -> 203 0.03635

193 -> 207 -0.02994

193 -> 212 -0.01248

193 -> 247 0.00118

193 -> 318 0.00133

193 -> 335 -0.00227

194 -> 204 0.03635

194 -> 208 -0.02994

194 -> 211 -0.01248

194 -> 248 -0.00118

194 -> 319 0.00133

194 -> 336 -0.00227

195 -> 206 0.03807

195 -> 221 0.00742

195 -> 245 0.00146

195 -> 325 -0.00216

195 -> 346 -0.00153

195 -> 415 0.00125

195 -> 514 -0.00111

196 -> 209 0.00550

196 -> 213 0.00193

196 -> 241 0.00217

196 -> 253 0.00181

196 -> 348 0.00108

196 -> 450 -0.00196

197 -> 210 -0.00161

197 -> 217 0.00138

197 -> 230 0.00289

197 -> 235 0.00125

197 -> 254 -0.00119

197 -> 280 0.00350

197 -> 285 0.00110

197 -> 303 0.00116

197 -> 314 0.00101

197 -> 349 0.00188

197 -> 366 0.00153

197 -> 378 -0.00108

197 -> 394 0.00123

197 -> 412 -0.00198

197 -> 433 -0.00155

197 -> 442 -0.00131

198 -> 210 -0.01371

198 -> 357 0.00112

199 -> 204 0.49616

199 -> 208 -0.00559

199 -> 211 0.00511

199 -> 262 -0.00337

200 -> 203 0.49616

200 -> 207 -0.00559

200 -> 212 0.00511

200 -> 261 0.00337

201 -> 205 0.01060

201 -> 223 -0.00427

201 -> 249 0.00126

201 -> 260 -0.00435

202 -> 210 -0.04253

202 -> 252 -0.00249

202 -> 259 0.00517

202 -> 357 0.00157

98 <- 290 0.00118

99 <- 284 0.00122

100 <- 283 -0.00122

104 <- 257 0.00102

104 <- 270 0.00111

104 <- 300 -0.00137

121 <- 258 -0.00101

121 <- 290 -0.00125

121 <- 311 0.00143

122 <- 284 -0.00149

122 <- 309 -0.00109

123 <- 283 -0.00149

123 <- 308 -0.00109

124 <- 286 0.00141

124 <- 293 -0.00129

124 <- 310 -0.00136

126 <- 230 0.00125

126 <- 254 0.00119

126 <- 266 0.00132

126 <- 289 -0.00135

126 <- 326 0.00109

126 <- 343 -0.00112

127 <- 255 -0.00110

127 <- 264 -0.00128

127 <- 279 0.00104

128 <- 256 -0.00110

128 <- 263 -0.00128

128 <- 278 0.00104

133 <- 234 -0.00146

133 <- 267 -0.00147

134 <- 205 0.00117

137 <- 210 -0.00109

138 <- 209 -0.00101

139 <- 257 0.00100

143 <- 203 -0.00208

143 <- 318 -0.00119

144 <- 204 -0.00208

144 <- 319 -0.00119

145 <- 277 0.00113

145 <- 286 -0.00152

145 <- 310 0.00105

145 <- 338 -0.00123

149 <- 206 -0.00276

154 <- 227 0.00100

154 <- 234 0.00189

154 <- 242 -0.00101

154 <- 258 -0.00209

154 <- 267 0.00133

154 <- 290 -0.00153

154 <- 311 0.00137

154 <- 332 -0.00124

154 <- 386 -0.00101

155 <- 239 0.00106

155 <- 243 -0.00132

155 <- 264 0.00190

155 <- 273 -0.00119

155 <- 282 -0.00137

155 <- 284 0.00107

155 <- 312 0.00122

156 <- 240 -0.00106

156 <- 244 0.00132

156 <- 263 -0.00190

156 <- 274 0.00119

156 <- 281 0.00137

156 <- 283 -0.00107

156 <- 313 -0.00122

157 <- 230 0.00103

157 <- 266 0.00236

157 <- 289 -0.00134

157 <- 343 -0.00188

158 <- 232 -0.00106

158 <- 269 0.00210

158 <- 291 0.00127

158 <- 301 0.00146

158 <- 308 0.00129

159 <- 233 -0.00106

159 <- 268 0.00210

159 <- 292 0.00127

159 <- 302 -0.00146

159 <- 309 0.00129

160 <- 246 0.00196

160 <- 265 0.00152

160 <- 277 -0.00118

160 <- 293 0.00318

160 <- 310 0.00145

160 <- 328 0.00107

161 <- 227 0.00136

161 <- 267 0.00115

161 <- 275 -0.00125

161 <- 290 0.00201

161 <- 311 -0.00154

162 <- 205 -0.00251

162 <- 339 0.00151

163 <- 270 0.00178

163 <- 276 -0.00138

163 <- 300 -0.00183

163 <- 315 0.00115

163 <- 337 0.00141

164 <- 209 -0.00183

164 <- 213 0.00130

165 <- 207 -0.00193

166 <- 208 -0.00193

168 <- 203 0.00397

168 <- 212 -0.00160

168 <- 261 -0.00136

169 <- 204 0.00397

169 <- 211 -0.00160

169 <- 262 0.00136

170 <- 210 -0.00243

170 <- 259 0.00147

171 <- 205 0.00621

171 <- 260 0.00150

171 <- 339 -0.00113

176 <- 283 0.00122

176 <- 291 0.00108

177 <- 284 0.00122

177 <- 292 0.00108

178 <- 266 -0.00120

179 <- 268 -0.00113

179 <- 284 0.00137

179 <- 292 -0.00108

180 <- 269 -0.00113

180 <- 283 0.00137

180 <- 291 -0.00108

181 <- 270 -0.00129

181 <- 300 0.00166

181 <- 337 -0.00135

182 <- 203 -0.00174

182 <- 207 -0.00529

182 <- 212 0.00131

182 <- 355 -0.00105

183 <- 204 0.00174

183 <- 208 0.00529

183 <- 211 -0.00131

183 <- 354 0.00105

184 <- 209 0.00192

188 <- 258 0.00121

188 <- 287 0.00102

188 <- 323 -0.00170

188 <- 347 -0.00113

188 <- 351 -0.00146

188 <- 440 -0.00169

189 <- 215 -0.00102

189 <- 264 -0.00119

189 <- 298 -0.00116

189 <- 353 0.00115

189 <- 362 0.00117

189 <- 447 0.00101

190 <- 214 -0.00102

190 <- 263 -0.00119

190 <- 299 -0.00116

190 <- 352 0.00115

190 <- 361 0.00117

190 <- 448 0.00101

191 <- 222 0.00141

191 <- 231 0.00155

191 <- 277 0.00158

191 <- 286 -0.00201

191 <- 338 -0.00102

192 <- 209 -0.01453

192 <- 213 0.00380

192 <- 271 0.00119

192 <- 327 0.00163

193 <- 203 0.00567

193 <- 207 -0.01311

193 <- 212 -0.00570

193 <- 335 -0.00150

194 <- 204 0.00567

194 <- 208 -0.01311

194 <- 211 -0.00570

194 <- 336 -0.00150

195 <- 206 0.01563

195 <- 221 0.00353

195 <- 325 -0.00146

195 <- 346 -0.00102

196 <- 209 0.00350

196 <- 241 0.00105

196 <- 450 -0.00164

197 <- 230 0.00150

197 <- 280 0.00224

197 <- 349 0.00137

197 <- 366 0.00115

197 <- 412 -0.00156

197 <- 433 -0.00122

197 <- 442 -0.00103

198 <- 210 -0.00332

198 <- 259 -0.00105

199 <- 204 -0.02454

199 <- 208 -0.00492

199 <- 211 0.00261

199 <- 238 -0.00166

199 <- 248 0.00108

199 <- 262 -0.00303

200 <- 203 -0.02454

200 <- 207 -0.00492

200 <- 212 0.00261

200 <- 237 0.00166

200 <- 247 -0.00108

200 <- 261 0.00303

201 <- 205 -0.01847

201 <- 249 0.00110

201 <- 260 -0.00327

202 <- 210 -0.01959

202 <- 252 -0.00118

202 <- 259 0.00476

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

65 -> 204 -0.00125

66 -> 223 0.00104

69 -> 203 -0.00180

70 -> 205 -0.00117

70 -> 223 0.00116

72 -> 204 -0.00111

97 -> 203 0.00233

105 -> 203 0.00330

105 -> 212 0.00131

112 -> 203 -0.00200

115 -> 205 0.00159

115 -> 223 -0.00154

116 -> 206 0.00143

116 -> 221 -0.00155

125 -> 207 -0.00172

125 -> 237 0.00225

125 -> 239 0.00106

125 -> 247 -0.00134

142 -> 203 -0.00171

143 -> 205 0.00110

143 -> 223 -0.00120

144 -> 206 0.00157

144 -> 209 -0.00125

149 -> 204 0.00216

149 -> 208 -0.00108

154 -> 208 0.00128

154 -> 238 0.00109

155 -> 205 0.00122

155 -> 223 -0.00117

156 -> 206 -0.00112

157 -> 212 0.00120

159 -> 205 0.00138

161 -> 204 0.00140

161 -> 208 0.00119

161 -> 238 0.00127

162 -> 203 0.00312

163 -> 207 -0.00151

166 -> 206 0.00101

166 -> 221 -0.00143

167 -> 204 0.00323

170 -> 212 0.00104

171 -> 207 0.00110

171 -> 212 -0.00125

172 -> 208 -0.00204

172 -> 238 -0.00211

172 -> 248 0.00114

173 -> 206 -0.00175

173 -> 221 0.00199

174 -> 205 -0.00248

174 -> 210 0.00106

174 -> 223 0.00185

176 -> 206 -0.00433

176 -> 209 0.00179

176 -> 221 0.00325

176 -> 241 0.00110

177 -> 205 -0.00738

177 -> 210 0.00149

177 -> 223 0.00438

178 -> 203 -0.01602

178 -> 207 0.00118

178 -> 212 -0.00393

179 -> 205 -0.00469

179 -> 210 -0.00177

180 -> 206 -0.00156

181 -> 203 0.00319

181 -> 207 0.00215

181 -> 212 -0.00108

182 -> 205 -0.00460

182 -> 210 -0.00232

183 -> 206 -0.00140

183 -> 209 -0.00128

183 -> 221 0.00177

183 -> 258 -0.00107

184 -> 204 -0.00238

185 -> 204 0.00155

185 -> 208 -0.00103

188 -> 208 0.01287

188 -> 211 -0.00214

188 -> 238 0.00780

188 -> 240 0.00364

188 -> 248 -0.00461

188 -> 250 -0.00106

188 -> 262 -0.00152

188 -> 477 -0.00129

189 -> 205 0.05437

189 -> 210 -0.00511

189 -> 223 -0.01581

189 -> 260 -0.00203

189 -> 472 0.00160

190 -> 206 0.02928

190 -> 209 -0.00648

190 -> 213 -0.00132

190 -> 218 0.00153

190 -> 221 -0.01655

190 -> 241 -0.00333

190 -> 245 -0.00139

190 -> 253 -0.00323

190 -> 271 0.00148

190 -> 450 0.00200

191 -> 204 -0.00114

192 -> 204 -0.00357

192 -> 208 0.00426

192 -> 211 0.00223

192 -> 238 -0.00106

193 -> 205 0.00282

193 -> 223 -0.00101

194 -> 206 -0.00452

194 -> 209 0.00432

194 -> 213 -0.00175

194 -> 221 -0.00276

194 -> 241 -0.00102

194 -> 253 -0.00131

195 -> 204 0.01015

195 -> 208 0.00361

195 -> 211 0.00342

195 -> 238 -0.00107

196 -> 204 -0.09075

196 -> 208 0.00159

196 -> 211 -0.00422

196 -> 281 0.00112

197 -> 203 0.63703

197 -> 207 -0.00831

197 -> 212 0.02255

197 -> 237 -0.00186

197 -> 239 -0.00103

197 -> 261 0.00193

197 -> 438 -0.00181

197 -> 476 0.00145

198 -> 203 -0.28249

198 -> 207 0.00199

198 -> 212 -0.00477

199 -> 206 -0.00205

199 -> 209 0.00165

199 -> 221 0.00107

200 -> 205 0.00332

200 -> 210 -0.00199

200 -> 223 -0.00132

200 -> 259 0.00101

200 -> 260 -0.00115

201 -> 203 0.00372

201 -> 207 -0.00156

201 -> 261 0.00118

202 -> 203 0.00408

202 -> 207 -0.00157

202 -> 212 0.00447

162 <- 203 0.00144

172 <- 204 0.00109

183 <- 258 -0.00101

183 <- 287 -0.00164

183 <- 367 -0.00103

188 <- 204 -0.00416

188 <- 208 -0.00131

188 <- 211 -0.00109

188 <- 238 -0.00216

188 <- 240 -0.00113

188 <- 248 0.00124

188 <- 262 0.00114

189 <- 205 -0.00437

189 <- 223 0.00349

189 <- 260 0.00120

190 <- 209 0.00179

190 <- 241 0.00185

190 <- 253 0.00176

190 <- 271 -0.00115

192 <- 208 0.00166

192 <- 211 0.00119

194 <- 206 -0.00124

194 <- 209 0.00168

194 <- 221 -0.00154

195 <- 208 0.00137

195 <- 211 0.00131

196 <- 204 -0.00435

196 <- 211 -0.00115

196 <- 269 -0.00141

196 <- 278 0.00197

196 <- 283 -0.00107

196 <- 299 0.00108

197 <- 203 -0.00547

197 <- 207 -0.00103

197 <- 212 -0.00141

197 <- 237 0.00215

197 <- 247 -0.00120

197 <- 261 -0.00122

198 <- 203 0.00325

198 <- 292 -0.00108

200 <- 205 -0.00278

200 <- 210 -0.00163

201 <- 203 -0.00186

201 <- 207 -0.00150

202 <- 207 -0.00106

202 <- 212 0.00197

202 <- 279 -0.00163

202 <- 284 0.00111

202 <- 292 -0.00177

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

65 -> 203 -0.00125

67 -> 223 0.00104

69 -> 204 -0.00180

71 -> 205 -0.00117

71 -> 223 0.00116

72 -> 203 -0.00111

97 -> 204 0.00233

105 -> 204 0.00330

105 -> 211 0.00131

112 -> 204 -0.00200

115 -> 206 -0.00143

115 -> 221 0.00155

116 -> 205 0.00159

116 -> 223 -0.00154

125 -> 208 0.00172

125 -> 238 0.00225

125 -> 240 0.00106

125 -> 248 -0.00134

142 -> 204 -0.00171

143 -> 206 0.00157

143 -> 209 0.00125

144 -> 205 -0.00110

144 -> 223 0.00120

149 -> 203 0.00216

149 -> 207 -0.00108

154 -> 207 0.00128

154 -> 237 -0.00109

155 -> 206 -0.00112

156 -> 205 -0.00122

156 -> 223 0.00117

157 -> 211 0.00120

158 -> 205 0.00138

161 -> 203 0.00140

161 -> 207 0.00119

161 -> 237 -0.00127

162 -> 204 -0.00312

163 -> 208 0.00151

165 -> 206 0.00101

165 -> 221 -0.00143

167 -> 203 0.00323

170 -> 211 0.00104

171 -> 208 -0.00110

171 -> 211 0.00125

172 -> 207 -0.00204

172 -> 237 0.00211

172 -> 247 -0.00114

173 -> 205 -0.00248

173 -> 210 -0.00106

173 -> 223 0.00185

174 -> 206 0.00175

174 -> 221 -0.00199

176 -> 205 -0.00738

176 -> 210 -0.00149

176 -> 223 0.00438

177 -> 206 0.00433

177 -> 209 0.00179

177 -> 221 -0.00325

177 -> 241 0.00110

178 -> 204 -0.01602

178 -> 208 0.00118

178 -> 211 -0.00393

179 -> 206 0.00156

180 -> 205 -0.00469

180 -> 210 0.00177

181 -> 204 -0.00319

181 -> 208 -0.00215

181 -> 211 0.00108

182 -> 206 0.00140

182 -> 209 -0.00128

182 -> 221 -0.00177

182 -> 258 0.00107

183 -> 205 -0.00460

183 -> 210 0.00232

184 -> 203 0.00238

185 -> 203 0.00155

185 -> 207 -0.00103

188 -> 207 0.01287

188 -> 212 -0.00214

188 -> 237 -0.00780

188 -> 239 -0.00364

188 -> 247 0.00461

188 -> 251 -0.00106

188 -> 261 0.00152

188 -> 476 0.00129

189 -> 206 -0.02928

189 -> 209 -0.00648

189 -> 213 -0.00132

189 -> 218 -0.00153

189 -> 221 0.01655

189 -> 241 -0.00333

189 -> 245 0.00139

189 -> 253 -0.00323

189 -> 271 0.00148

189 -> 450 0.00200

190 -> 205 0.05437

190 -> 210 0.00511

190 -> 223 -0.01581

190 -> 260 -0.00203

190 -> 472 0.00160

191 -> 203 0.00114

192 -> 203 0.00357

192 -> 207 -0.00426

192 -> 212 -0.00223

192 -> 237 -0.00106

193 -> 206 -0.00452

193 -> 209 -0.00432

193 -> 213 0.00175

193 -> 221 -0.00276

193 -> 241 0.00102

193 -> 253 0.00131

194 -> 205 -0.00282

194 -> 223 0.00101

195 -> 203 0.01015

195 -> 207 0.00361

195 -> 212 0.00342

195 -> 237 0.00107

196 -> 203 0.09075

196 -> 207 -0.00159

196 -> 212 0.00422

196 -> 282 0.00112

197 -> 204 0.63703

197 -> 208 -0.00831

197 -> 211 0.02255

197 -> 238 0.00186

197 -> 240 0.00103

197 -> 262 -0.00193

197 -> 439 -0.00181

197 -> 477 -0.00145

198 -> 204 -0.28249

198 -> 208 0.00199

198 -> 211 -0.00477

199 -> 205 -0.00332

199 -> 210 -0.00199

199 -> 223 0.00132

199 -> 259 0.00101

199 -> 260 0.00115

200 -> 206 -0.00205

200 -> 209 -0.00165

200 -> 221 0.00107

201 -> 204 -0.00372

201 -> 208 0.00156

201 -> 262 0.00118

202 -> 204 0.00408

202 -> 208 -0.00157

202 -> 211 0.00447

162 <- 204 -0.00144

172 <- 203 0.00109

182 <- 258 0.00101

182 <- 287 0.00164

182 <- 367 0.00103

188 <- 203 -0.00416

188 <- 207 -0.00131

188 <- 212 -0.00109

188 <- 237 0.00216

188 <- 239 0.00113

188 <- 247 -0.00124

188 <- 261 -0.00114

189 <- 209 0.00179

189 <- 241 0.00185

189 <- 253 0.00176

189 <- 271 -0.00115

190 <- 205 -0.00437

190 <- 223 0.00349

190 <- 260 0.00120

192 <- 207 -0.00166

192 <- 212 -0.00119

193 <- 206 -0.00124

193 <- 209 -0.00168

193 <- 221 -0.00154

195 <- 207 0.00137

195 <- 212 0.00131

196 <- 203 0.00435

196 <- 212 0.00115

196 <- 268 -0.00141

196 <- 279 0.00197

196 <- 284 -0.00107

196 <- 298 0.00108

197 <- 204 -0.00547

197 <- 208 -0.00103

197 <- 211 -0.00141

197 <- 238 -0.00215

197 <- 248 0.00120

197 <- 262 0.00122

198 <- 204 0.00325

198 <- 291 0.00108

199 <- 205 0.00278

199 <- 210 -0.00163

201 <- 204 0.00186

201 <- 208 0.00150

202 <- 208 -0.00106

202 <- 211 0.00197

202 <- 278 0.00163

202 <- 283 -0.00111

202 <- 291 0.00177

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

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

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

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(A2)

The electronic state is 1-A1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Alpha occ. eigenvalues -- -0.20666 -0.16896

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

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

Alpha virt. eigenvalues -- 0.04107 0.05049 0.05049 0.05129 0.05446

Alpha virt. eigenvalues -- 0.05861 0.06071 0.06071 0.06305 0.06444

Alpha virt. eigenvalues -- 0.06491 0.06937 0.06937 0.07960 0.08108

Alpha virt. eigenvalues -- 0.09322 0.09322 0.09923 0.11112 0.11325

Alpha virt. eigenvalues -- 0.11325 0.11539 0.11570 0.11734 0.11767

Alpha virt. eigenvalues -- 0.11767 0.11785 0.11785 0.12142 0.12702

Alpha virt. eigenvalues -- 0.12861 0.12861 0.12969 0.13144 0.13200

Alpha virt. eigenvalues -- 0.13200 0.13254 0.13326 0.13326 0.13372

Alpha virt. eigenvalues -- 0.13477 0.16949 0.16984 0.16984 0.17011

Alpha virt. eigenvalues -- 0.17593 0.18565 0.18888 0.18997 0.18997

Alpha virt. eigenvalues -- 0.20418 0.20418 0.20484 0.20715 0.20989

Alpha virt. eigenvalues -- 0.21449 0.21449 0.22002 0.22304 0.22821

Alpha virt. eigenvalues -- 0.23609 0.23609 0.24252 0.24662 0.24691

Alpha virt. eigenvalues -- 0.24981 0.24981 0.25130 0.25837 0.25837

Alpha virt. eigenvalues -- 0.26312 0.26312 0.26647 0.27787 0.28613

Alpha virt. eigenvalues -- 0.28824 0.29310 0.29813 0.30191 0.30191

Alpha virt. eigenvalues -- 0.30345 0.31079 0.31082 0.31082 0.31274

Alpha virt. eigenvalues -- 0.31489 0.31489 0.32404 0.32622 0.32622

Alpha virt. eigenvalues -- 0.33322 0.33672 0.33730 0.33730 0.33800

Alpha virt. eigenvalues -- 0.34790 0.34790 0.34803 0.35138 0.35343

Alpha virt. eigenvalues -- 0.35343 0.36017 0.36104 0.36925 0.36925

Alpha virt. eigenvalues -- 0.37337 0.37337 0.37910 0.38168 0.38168

Alpha virt. eigenvalues -- 0.38271 0.38406 0.38575 0.38771 0.39263

Alpha virt. eigenvalues -- 0.39366 0.39532 0.39828 0.39828 0.39959

Alpha virt. eigenvalues -- 0.40011 0.40011 0.40848 0.40848 0.41201

Alpha virt. eigenvalues -- 0.41318 0.41674 0.41922 0.41922 0.42196

Alpha virt. eigenvalues -- 0.43000 0.43458 0.43458 0.43649 0.43824

Alpha virt. eigenvalues -- 0.43998 0.44420 0.44459 0.44496 0.44543

Alpha virt. eigenvalues -- 0.44543 0.45350 0.45350 0.46313 0.46384

Alpha virt. eigenvalues -- 0.46428 0.46428 0.46995 0.48304 0.48304

Alpha virt. eigenvalues -- 0.48588 0.48588 0.49121 0.49168 0.49241

Alpha virt. eigenvalues -- 0.49503 0.49601 0.49601 0.50292 0.50292

Alpha virt. eigenvalues -- 0.50327 0.50330 0.50343 0.50585 0.50585

Alpha virt. eigenvalues -- 0.51294 0.51884 0.52565 0.52565 0.52705

Alpha virt. eigenvalues -- 0.52705 0.52870 0.53319 0.53372 0.53614

Alpha virt. eigenvalues -- 0.54420 0.54700 0.55225 0.55225 0.55700

Alpha virt. eigenvalues -- 0.55700 0.56153 0.56914 0.57268 0.57268

Alpha virt. eigenvalues -- 0.57680 0.57700 0.58104 0.58104 0.58531

Alpha virt. eigenvalues -- 0.58723 0.58723 0.59219 0.59307 0.59483

Alpha virt. eigenvalues -- 0.59967 0.59967 0.60333 0.61306 0.61393

Alpha virt. eigenvalues -- 0.61784 0.61784 0.62015 0.62663 0.62663

Alpha virt. eigenvalues -- 0.63131 0.63202 0.63311 0.63588 0.63674

Alpha virt. eigenvalues -- 0.63674 0.63912 0.63912 0.64278 0.64278

Alpha virt. eigenvalues -- 0.64454 0.64941 0.65013 0.65013 0.65124

Alpha virt. eigenvalues -- 0.65216 0.65716 0.65789 0.65889 0.65889

Alpha virt. eigenvalues -- 0.67509 0.67509 0.67700 0.67702 0.69277

Alpha virt. eigenvalues -- 0.69798 0.69798 0.70430 0.70720 0.70995

Alpha virt. eigenvalues -- 0.70995 0.72276 0.72393 0.72693 0.72755

Alpha virt. eigenvalues -- 0.72755 0.73031 0.73031 0.73638 0.75361

Alpha virt. eigenvalues -- 0.75361 0.75988 0.76354 0.76747 0.77548

Alpha virt. eigenvalues -- 0.77548 0.78373 0.78591 0.78785 0.78804

Alpha virt. eigenvalues -- 0.78882 0.78882 0.79099 0.79995 0.80846

Alpha virt. eigenvalues -- 0.81383 0.81396 0.81396 0.81559 0.81559

Alpha virt. eigenvalues -- 0.82502 0.83140 0.83175 0.83175 0.83696

Alpha virt. eigenvalues -- 0.83696 0.84371 0.85132 0.85450 0.85570

Alpha virt. eigenvalues -- 0.85570 0.85834 0.86367 0.86670 0.87651

Alpha virt. eigenvalues -- 0.87651 0.87687 0.88526 0.88526 0.88678

Alpha virt. eigenvalues -- 0.90499 0.91621 0.91621 0.91900 0.92217

Alpha virt. eigenvalues -- 0.92217 0.93391 0.93717 0.93803 0.94049

Alpha virt. eigenvalues -- 0.94049 0.95081 0.95081 0.95549 0.95558

Alpha virt. eigenvalues -- 0.96314 0.96814 0.97125 0.98312 0.98312

Alpha virt. eigenvalues -- 0.98654 0.98654 0.98858 0.99274 0.99295

Alpha virt. eigenvalues -- 0.99295 0.99851 1.00230 1.02368 1.02368

Alpha virt. eigenvalues -- 1.03127 1.03341 1.04372 1.04996 1.04996

Alpha virt. eigenvalues -- 1.07550 1.07550 1.08028 1.08028 1.08042

Alpha virt. eigenvalues -- 1.08081 1.08332 1.08355 1.09459 1.11503

Alpha virt. eigenvalues -- 1.11546 1.11546 1.11611 1.11761 1.11843

Alpha virt. eigenvalues -- 1.12200 1.12200 1.13088 1.14098 1.14098

Alpha virt. eigenvalues -- 1.14189 1.14330 1.14330 1.15433 1.15984

Alpha virt. eigenvalues -- 1.17756 1.18191 1.18191 1.18461 1.18946

Alpha virt. eigenvalues -- 1.19375 1.19375 1.19565 1.19682 1.19682

Alpha virt. eigenvalues -- 1.19967 1.22238 1.22402 1.23612 1.23673

Alpha virt. eigenvalues -- 1.23770 1.23790 1.23790 1.24103 1.24103

Alpha virt. eigenvalues -- 1.25528 1.25528 1.26277 1.27204 1.27204

Alpha virt. eigenvalues -- 1.27498 1.27996 1.28039 1.28498 1.30165

Alpha virt. eigenvalues -- 1.30662 1.31695 1.31894 1.31894 1.33481

Alpha virt. eigenvalues -- 1.33591 1.33591 1.33730 1.34526 1.34909

Alpha virt. eigenvalues -- 1.34909 1.35394 1.35720 1.36267 1.36267

Alpha virt. eigenvalues -- 1.37733 1.38282 1.38282 1.38405 1.39400

Alpha virt. eigenvalues -- 1.41037 1.41928 1.43943 1.43943 1.44782

Alpha virt. eigenvalues -- 1.44782 1.46388 1.47683 1.47683 1.48266

Alpha virt. eigenvalues -- 1.48322 1.48660 1.48660 1.50384 1.50384

Alpha virt. eigenvalues -- 1.50397 1.50583 1.51255 1.51550 1.51550

Alpha virt. eigenvalues -- 1.51646 1.51797 1.52001 1.52497 1.52595

Alpha virt. eigenvalues -- 1.52785 1.52859 1.52859 1.52978 1.52978

Alpha virt. eigenvalues -- 1.53092 1.53259 1.54266 1.54266 1.54655

Alpha virt. eigenvalues -- 1.55597 1.55965 1.56286 1.56286 1.56529

Alpha virt. eigenvalues -- 1.56718 1.56718 1.57920 1.57920 1.58591

Alpha virt. eigenvalues -- 1.59033 1.59640 1.59640 1.59643 1.59792

Alpha virt. eigenvalues -- 1.61043 1.61311 1.61830 1.61830 1.62446

Alpha virt. eigenvalues -- 1.64410 1.64410 1.64617 1.64617 1.64754

Alpha virt. eigenvalues -- 1.66535 1.66535 1.67016 1.68655 1.69049

Alpha virt. eigenvalues -- 1.69094 1.69643 1.69643 1.70359 1.71146

Alpha virt. eigenvalues -- 1.71215 1.71964 1.71964 1.72456 1.74038

Alpha virt. eigenvalues -- 1.74038 1.74600 1.75150 1.75407 1.75407

Alpha virt. eigenvalues -- 1.75502 1.77555 1.77555 1.77713 1.78867

Alpha virt. eigenvalues -- 1.79136 1.79568 1.80026 1.80026 1.80147

Alpha virt. eigenvalues -- 1.80147 1.80539 1.80966 1.81177 1.82014

Alpha virt. eigenvalues -- 1.82014 1.82252 1.84198 1.84198 1.84328

Alpha virt. eigenvalues -- 1.85543 1.87405 1.88031 1.88158 1.88158

Alpha virt. eigenvalues -- 1.89180 1.89286 1.89286 1.89384 1.90494

Alpha virt. eigenvalues -- 1.90673 1.90673 1.90794 1.90871 1.91191

Alpha virt. eigenvalues -- 1.91953 1.91953 1.95203 1.96362 1.96362

Alpha virt. eigenvalues -- 1.96493 1.97083 1.98383 1.98452 1.98452

Alpha virt. eigenvalues -- 1.99209 1.99299 1.99299 2.00030 2.01487

Alpha virt. eigenvalues -- 2.01730 2.01730 2.02692 2.03485 2.07975

Alpha virt. eigenvalues -- 2.08945 2.08999 2.09135 2.09258 2.09258

Alpha virt. eigenvalues -- 2.10109 2.11316 2.11316 2.13550 2.13550

Alpha virt. eigenvalues -- 2.14628 2.15639 2.16339 2.16339 2.18559

Alpha virt. eigenvalues -- 2.19721 2.20806 2.20806 2.21423 2.22291

Alpha virt. eigenvalues -- 2.24182 2.24254 2.25636 2.25636 2.25730

Alpha virt. eigenvalues -- 2.25730 2.26658 2.27461 2.27952 2.28358

Alpha virt. eigenvalues -- 2.28358 2.28541 2.30059 2.30059 2.31218

Alpha virt. eigenvalues -- 2.31978 2.32005 2.33555 2.33555 2.34094

Alpha virt. eigenvalues -- 2.34200 2.34200 2.34304 2.34344 2.34519

Alpha virt. eigenvalues -- 2.34657 2.34657 2.34736 2.35190 2.35284

Alpha virt. eigenvalues -- 2.36760 2.36760 2.37968 2.39356 2.39800

Alpha virt. eigenvalues -- 2.39800 2.40336 2.40336 2.40339 2.41410

Alpha virt. eigenvalues -- 2.43240 2.43597 2.43597 2.44116 2.44353

Alpha virt. eigenvalues -- 2.44353 2.45063 2.47556 2.48798 2.48798

Alpha virt. eigenvalues -- 2.49592 2.50111 2.50564 2.51257 2.51257

Alpha virt. eigenvalues -- 2.51662 2.51662 2.51728 2.51824 2.54097

Alpha virt. eigenvalues -- 2.54789 2.56978 2.56978 2.58167 2.59071

Alpha virt. eigenvalues -- 2.59071 2.61379 2.62439 2.63062 2.64476

Alpha virt. eigenvalues -- 2.64476 2.64699 2.65142 2.67022 2.67022

Alpha virt. eigenvalues -- 2.67402 2.67402 2.67721 2.68057 2.68467

Alpha virt. eigenvalues -- 2.72792 2.73171 2.74096 2.74281 2.74281

Alpha virt. eigenvalues -- 2.74285 2.74622 2.74622 2.78111 2.78111

Alpha virt. eigenvalues -- 2.79141 2.79256 2.79733 2.80146 2.80146

Alpha virt. eigenvalues -- 2.81796 2.81942 2.81942 2.82068 2.83220

Alpha virt. eigenvalues -- 2.83429 2.83429 2.83841 2.84993 2.85619

Alpha virt. eigenvalues -- 2.86727 2.86938 2.86938 2.87132 2.87132

Alpha virt. eigenvalues -- 2.87545 2.87808 2.87808 2.89028 2.89227

Alpha virt. eigenvalues -- 2.90319 2.91151 2.94018 2.94018 2.94750

Alpha virt. eigenvalues -- 2.94871 2.95132 2.95132 2.96084 2.96268

Alpha virt. eigenvalues -- 2.98764 2.98764 2.99422 3.00515 3.00515

Alpha virt. eigenvalues -- 3.00831 3.00996 3.01748 3.02942 3.02942

Alpha virt. eigenvalues -- 3.03803 3.05070 3.06208 3.06208 3.06414

Alpha virt. eigenvalues -- 3.07922 3.07922 3.08917 3.11748 3.13121

Alpha virt. eigenvalues -- 3.13387 3.13387 3.13979 3.14115 3.14848

Alpha virt. eigenvalues -- 3.14848 3.15511 3.15884 3.16284 3.16427

Alpha virt. eigenvalues -- 3.16427 3.17612 3.17795 3.17795 3.18339

Alpha virt. eigenvalues -- 3.19344 3.19393 3.20304 3.20388 3.20388

Alpha virt. eigenvalues -- 3.20454 3.21215 3.21261 3.21261 3.21303

Alpha virt. eigenvalues -- 3.21563 3.21563 3.22011 3.22359 3.22359

Alpha virt. eigenvalues -- 3.23327 3.24933 3.26407 3.26407 3.27005

Alpha virt. eigenvalues -- 3.28785 3.28842 3.28842 3.29147 3.29227

Alpha virt. eigenvalues -- 3.30447 3.30447 3.31320 3.31422 3.32987

Alpha virt. eigenvalues -- 3.32987 3.35669 3.37154 3.37576 3.38167

Alpha virt. eigenvalues -- 3.38167 3.41075 3.41075 3.41216 3.41316

Alpha virt. eigenvalues -- 3.41509 3.42051 3.42051 3.43262 3.45569

Alpha virt. eigenvalues -- 3.47203 3.47203 3.49013 3.55631 3.60857

Alpha virt. eigenvalues -- 3.60857 3.61368 3.61970 3.62685 3.62685

Alpha virt. eigenvalues -- 3.67814 3.68015 3.68015 3.68769 3.76619

Alpha virt. eigenvalues -- 3.76926 3.77999 3.77999 3.78833 3.80124

Alpha virt. eigenvalues -- 3.80124 3.81311 3.82890 3.82890 3.83043

Alpha virt. eigenvalues -- 3.84845 3.87215 3.89364 3.89535 3.89535

Alpha virt. eigenvalues -- 3.92111 3.95742 3.96880 3.96880 3.97741

Alpha virt. eigenvalues -- 3.98613 3.98613 3.98917 3.99600 4.01922

Alpha virt. eigenvalues -- 4.01922 4.02579 4.02641 4.11584 4.15126

Alpha virt. eigenvalues -- 4.15126 4.17185 4.18203 4.18203 4.19775

Alpha virt. eigenvalues -- 4.21838 4.23261 4.24626 4.24626 4.27271

Alpha virt. eigenvalues -- 4.35398 4.41755 4.41755 4.42486 4.46963

Alpha virt. eigenvalues -- 4.52114 4.61512 4.61512 4.82427 4.82429

Alpha virt. eigenvalues -- 4.82429 4.82576 4.87818 4.88250 4.88250

Alpha virt. eigenvalues -- 4.89138 4.89179 4.89852 4.89852 4.90121

Alpha virt. eigenvalues -- 5.13633 5.13642 5.13642 5.17251 5.21812

Alpha virt. eigenvalues -- 5.25966 5.26628 5.26628 5.27311 5.29964

Alpha virt. eigenvalues -- 5.30289 5.30289 5.31285 5.38394 5.38394

Alpha virt. eigenvalues -- 5.56086 5.67529 5.69050 5.69050 5.69387

Alpha virt. eigenvalues -- 5.75818 5.76216 5.76216 5.77002 7.77599

Alpha virt. eigenvalues -- 7.77599 7.88709 7.95021 8.20751 11.17031

Alpha virt. eigenvalues -- 23.34464 23.37771 23.37771 23.39775 23.44693

Alpha virt. eigenvalues -- 23.45091 23.45091 23.45571 23.46199 23.46424

Alpha virt. eigenvalues -- 23.46424 23.46555 23.77721 23.79473 23.79473

Alpha virt. eigenvalues -- 23.80893 23.82802 23.83201 23.83201 23.83532

Alpha virt. eigenvalues -- 23.88876 23.88876 23.89012 23.89254 23.89453

Alpha virt. eigenvalues -- 23.90784 23.90784 23.91003 24.02322 24.02329

Alpha virt. eigenvalues -- 24.02329 24.02440 24.03595 24.03885 24.03885

Alpha virt. eigenvalues -- 24.04443 24.11459 24.11489 24.11489 24.11630

Alpha virt. eigenvalues -- 35.58110 35.61417 35.61417 35.62327 35.70076

Alpha virt. eigenvalues -- 35.71260 35.71260 35.71424 49.92018 49.92454

Alpha virt. eigenvalues -- 49.92454 49.92730 49.92893 49.93264 49.93264

Alpha virt. eigenvalues -- 49.93495

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C 0.385494

2 N -0.687379

3 C 0.385494

4 C -0.092977

5 C -0.092977

6 N -0.342451

7 C 0.385494

8 N -0.687379

9 C 0.385494

10 C -0.092977

11 C -0.092977

12 N -0.342451

13 C -0.092977

14 C -0.092977

15 C 0.385494

16 N -0.687379

17 C 0.385494

18 N -0.342451

19 N -0.687379

20 C 0.385494

21 C -0.092977

22 C -0.092977

23 C 0.385494

24 N -0.342451

25 Zn 1.449984

26 C 0.202394

27 C -0.307078

28 C -0.307078

29 C 0.202394

30 C 0.202394

31 C -0.307078

32 C -0.307078

33 C 0.202394

34 C 0.202394

35 C -0.307078

36 C -0.307078

37 C 0.202394

38 C 0.202394

39 C -0.307078

40 C -0.307078

41 C 0.202394

42 H 0.255919

43 H 0.255919

44 H 0.255919

45 H 0.255919

46 H 0.255919

47 H 0.255919

48 H 0.255919

49 H 0.255919

50 O -0.315694

51 O -0.315694

52 O -0.315694

53 O -0.315694

54 O -0.315694

55 O -0.315694

56 O -0.315694

57 O -0.315694

58 C -0.505457

59 H 0.227146

60 H 0.256628

61 C -0.505457

62 H 0.227146

63 H 0.256628

64 C -0.505457

65 H 0.227146

66 H 0.256628

67 C -0.505457

68 H 0.227146

69 H 0.256628

70 C -0.505457

71 H 0.227146

72 H 0.256628

73 C -0.505457

74 H 0.227146

75 H 0.256628

76 C -0.505457

77 H 0.227146

78 H 0.256628

79 C -0.505457

80 H 0.227146

81 H 0.256628

82 H 0.227293

83 H 0.227293

84 H 0.227293

85 H 0.227293

86 H 0.227293

87 H 0.227293

88 H 0.227293

89 H 0.227293

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.385494

2 N -0.687379

3 C 0.385494

4 C -0.092977

5 C -0.092977

6 N -0.342451

7 C 0.385494

8 N -0.687379

9 C 0.385494

10 C -0.092977

11 C -0.092977

12 N -0.342451

13 C -0.092977

14 C -0.092977

15 C 0.385494

16 N -0.687379

17 C 0.385494

18 N -0.342451

19 N -0.687379

20 C 0.385494

21 C -0.092977

22 C -0.092977

23 C 0.385494

24 N -0.342451

25 Zn 1.449984

26 C 0.202394

27 C -0.051160

28 C -0.051160

29 C 0.202394

30 C 0.202394

31 C -0.051160

32 C -0.051160

33 C 0.202394

34 C 0.202394

35 C -0.051160

36 C -0.051160

37 C 0.202394

38 C 0.202394

39 C -0.051160

40 C -0.051160

41 C 0.202394

50 O -0.315694

51 O -0.315694

52 O -0.315694

53 O -0.315694

54 O -0.315694

55 O -0.315694

56 O -0.315694

57 O -0.315694

58 C 0.205610

61 C 0.205610

64 C 0.205610

67 C 0.205610

70 C 0.205610

73 C 0.205610

76 C 0.205610

79 C 0.205610

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

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

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

XY= 0.0000 XZ= -0.0000 YZ= 0.0000

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

XX= 45.6869 YY= 45.6869 ZZ= -91.3738

XY= 0.0000 XZ= -0.0000 YZ= 0.0000

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

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

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

YYZ= 16.6252 XYZ= -0.0000

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

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

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

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

XXYZ= 0.0000 YYXZ= -0.0000 ZZXY= 0.0000

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

Symmetry A1 KE= 7.472512070613D+02

Symmetry A2 KE= 6.108286470496D+02

Symmetry B1 KE= 6.660088939415D+02

Symmetry B2 KE= 6.660088939415D+02

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

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

Test job not archived.

1\1\ WCSS.PL-BEM-DHCP-129-94-98-136\SP\RB3LYP TD-FC\GenECP\C40H32N8O8Z

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

46,-0.099713\C,0,-3.514352,6.580615,0.1027\H,0,-3.303559,7.194357,-0.7

78514\H,0,-4.56446,6.293917,0.099713\C,0,-6.580615,3.514352,-0.1027\H,

0,-7.194357,3.303559,0.778514\H,0,-6.293917,4.56446,-0.099713\C,0,-6.5

80615,-3.514352,-0.1027\H,0,-7.194357,-3.303559,0.778514\H,0,-6.293917

,-4.56446,-0.099713\C,0,-3.514352,-6.580615,0.1027\H,0,-3.303559,-7.19

4357,-0.778514\H,0,-4.56446,-6.293917,0.099713\C,0,3.514352,-6.580615,

0.1027\H,0,3.303559,-7.194357,-0.778514\H,0,4.56446,-6.293917,0.099713

\H,0,3.298342,-7.155737,1.008335\H,0,-3.298342,-7.155737,1.008335\H,0,

-7.155737,-3.298342,-1.008335\H,0,-7.155737,3.298342,-1.008335\H,0,3.2

98342,7.155737,1.008335\H,0,-3.298342,7.155737,1.008335\H,0,7.155737,-

3.298342,-1.008335\H,0,7.155737,3.298342,-1.008335\\Version=ES64L-G09R

evE.01\State=1-A1\HF=-2649.8283939\RMSD=4.396e-09\PG=D02D [O(Zn1),2SGD

(N2),X(C40H32N4O8)]\\@

A people that values its privileges above its principles soon loses both.

-- Dwight D. Eisenhower

Job cpu time: 0 days 4 hours 45 minutes 24.8 seconds.

File lengths (MBytes): RWF= 4848 Int= 0 D2E= 0 Chk= 488 Scr= 1

Normal termination of Gaussian 09 at Thu Sep 19 01:09:03 2019.