Entering Gaussian System, Link 0=g09

Input=ZnNPC0td.com

Output=ZnNPC0td.log

Initial command:

/home/blab/g09/l1.exe "/home/blab/g09/scratch/Gau-46585.inp" -scrdir="/home/blab/g09/scratch/"

Entering Link 1 = /home/blab/g09/l1.exe PID= 46593.

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

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

Cite this work as:

Gaussian 09, Revision E.01,

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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=ZnNPC0td.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 00:35:28 2019, MaxMem= 1342177280 cpu: 40.7

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

--------

ZnNPC0td

--------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C 1.12208 2.79302 0.17278

N 0. 2.02036 0.25982

C -1.12208 2.79302 0.17278

C -0.71452 4.19463 0.05147

C 0.71452 4.19463 0.05147

N -2.38951 2.38951 0.15461

C -2.79302 1.12208 0.1728

N -2.02036 0. 0.25983

C -2.79302 -1.12208 0.1728

C -4.19464 -0.71452 0.05153

C -4.19464 0.71452 0.05153

N 2.38951 2.38951 0.15461

C 4.19464 0.71452 0.05153

C 4.19464 -0.71452 0.05153

C 2.79302 -1.12208 0.1728

N 2.02036 0. 0.25983

C 2.79302 1.12208 0.1728

N 2.38951 -2.38951 0.15461

N 0. -2.02036 0.25982

C 1.12208 -2.79302 0.17278

C 0.71452 -4.19463 0.05147

C -0.71452 -4.19463 0.05147

C -1.12208 -2.79302 0.17278

N -2.38951 -2.38951 0.15461

Zn 0. 0. 0.77753

C 5.36349 1.42745 -0.05462

C 6.58861 0.72073 -0.15638

C 6.58861 -0.72073 -0.15638

C 5.36349 -1.42745 -0.05462

C -1.42745 -5.36348 -0.05471

C -0.72073 -6.5886 -0.1565

C 0.72073 -6.5886 -0.1565

C 1.42745 -5.36348 -0.05471

C -5.36349 1.42745 -0.05462

C -6.58861 0.72073 -0.15638

C -6.58861 -0.72073 -0.15638

C -5.36349 -1.42745 -0.05462

C 1.42745 5.36348 -0.05471

C 0.72073 6.5886 -0.1565

C -0.72073 6.5886 -0.1565

C -1.42745 5.36348 -0.05471

C 1.40241 -7.83042 -0.25896

C 0.70807 -9.01151 -0.35678

C -0.70807 -9.01151 -0.35678

C -1.40241 -7.83042 -0.25896

C 7.83043 -1.40241 -0.2588

C 9.01152 -0.70807 -0.35659

C 9.01152 0.70807 -0.35659

C 7.83043 1.40241 -0.2588

C -1.40241 7.83042 -0.25896

C -0.70807 9.01151 -0.35678

C 0.70807 9.01151 -0.35678

C 1.40241 7.83042 -0.25896

C -7.83043 -1.40241 -0.2588

C -9.01152 -0.70807 -0.35659

C -9.01152 0.70807 -0.35659

C -7.83043 1.40241 -0.2588

H 5.36498 2.51242 -0.05821

H 5.36498 -2.51242 -0.05821

H -2.51242 -5.36498 -0.0583

H 2.51242 -5.36498 -0.0583

H -5.36498 2.51242 -0.05821

H -5.36498 -2.51242 -0.05821

H 2.51242 5.36498 -0.0583

H -2.51242 5.36498 -0.0583

H 2.48784 -7.82854 -0.25881

H 1.24326 -9.95179 -0.43509

H -1.24326 -9.95179 -0.43509

H -2.48784 -7.82854 -0.25881

H 7.82856 -2.48784 -0.25866

H 9.95181 -1.24326 -0.43487

H 9.95181 1.24326 -0.43487

H 7.82856 2.48784 -0.25866

H -2.48784 7.82854 -0.25881

H -1.24326 9.95179 -0.43509

H 1.24326 9.95179 -0.43509

H 2.48784 7.82854 -0.25881

H -7.82856 -2.48784 -0.25866

H -9.95181 -1.24326 -0.43487

H -9.95181 1.24326 -0.43487

H -7.82856 2.48784 -0.25866

NAtoms= 81 NQM= 81 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 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 51 52 53 54 55 56 57 58 59 60

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

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

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

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

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

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

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

Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

Atom 71 72 73 74 75 76 77 78 79 80

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

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

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

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

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

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

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

Atom 81

IAtWgt= 1

AtmWgt= 1.0078250

NucSpn= 1

AtZEff= 0.0000000

NQMom= 0.0000000

NMagM= 2.7928460

AtZNuc= 1.0000000

Leave Link 101 at Thu Sep 19 00:35:28 2019, MaxMem= 1342177280 cpu: 0.7

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

Stoichiometry C48H24N8Zn

Framework group C2V[C2(Zn),SGV(N2),SGV'(N2),X(C48H24N4)]

Deg. of freedom 61

Full point group C2V NOp 4

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 1.122077 2.793021 0.172784

2 7 0 0.000000 2.020361 0.259821

3 6 0 -1.122077 2.793021 0.172784

4 6 0 -0.714524 4.194635 0.051468

5 6 0 0.714524 4.194635 0.051468

6 7 0 -2.389506 2.389505 0.154613

7 6 0 -2.793023 1.122077 0.172801

8 7 0 -2.020362 0.000000 0.259826

9 6 0 -2.793023 -1.122077 0.172801

10 6 0 -4.194641 -0.714524 0.051526

11 6 0 -4.194641 0.714524 0.051526

12 7 0 2.389506 2.389505 0.154613

13 6 0 4.194641 0.714524 0.051526

14 6 0 4.194641 -0.714524 0.051526

15 6 0 2.793023 -1.122077 0.172801

16 7 0 2.020362 -0.000000 0.259826

17 6 0 2.793023 1.122077 0.172801

18 7 0 2.389506 -2.389505 0.154613

19 7 0 -0.000000 -2.020361 0.259821

20 6 0 1.122077 -2.793021 0.172784

21 6 0 0.714524 -4.194635 0.051468

22 6 0 -0.714524 -4.194635 0.051468

23 6 0 -1.122077 -2.793021 0.172784

24 7 0 -2.389506 -2.389505 0.154613

25 30 0 0.000000 0.000000 0.777528

26 6 0 5.363492 1.427454 -0.054616

27 6 0 6.588610 0.720730 -0.156377

28 6 0 6.588610 -0.720730 -0.156377

29 6 0 5.363492 -1.427454 -0.054616

30 6 0 -1.427454 -5.363483 -0.054708

31 6 0 -0.720730 -6.588598 -0.156501

32 6 0 0.720730 -6.588598 -0.156501

33 6 0 1.427454 -5.363483 -0.054708

34 6 0 -5.363492 1.427454 -0.054616

35 6 0 -6.588610 0.720730 -0.156377

36 6 0 -6.588610 -0.720730 -0.156377

37 6 0 -5.363492 -1.427454 -0.054616

38 6 0 1.427454 5.363483 -0.054708

39 6 0 0.720730 6.588598 -0.156501

40 6 0 -0.720730 6.588598 -0.156501

41 6 0 -1.427454 5.363483 -0.054708

42 6 0 1.402412 -7.830417 -0.258961

43 6 0 0.708074 -9.011507 -0.356784

44 6 0 -0.708074 -9.011507 -0.356784

45 6 0 -1.402412 -7.830417 -0.258961

46 6 0 7.830431 -1.402412 -0.258803

47 6 0 9.011524 -0.708074 -0.356593

48 6 0 9.011524 0.708074 -0.356593

49 6 0 7.830431 1.402412 -0.258803

50 6 0 -1.402412 7.830417 -0.258961

51 6 0 -0.708074 9.011507 -0.356784

52 6 0 0.708074 9.011507 -0.356784

53 6 0 1.402412 7.830417 -0.258961

54 6 0 -7.830431 -1.402412 -0.258803

55 6 0 -9.011524 -0.708074 -0.356593

56 6 0 -9.011524 0.708074 -0.356593

57 6 0 -7.830431 1.402412 -0.258803

58 1 0 5.364985 2.512421 -0.058211

59 1 0 5.364985 -2.512421 -0.058211

60 1 0 -2.512421 -5.364975 -0.058303

61 1 0 2.512421 -5.364975 -0.058303

62 1 0 -5.364985 2.512421 -0.058211

63 1 0 -5.364985 -2.512421 -0.058211

64 1 0 2.512421 5.364975 -0.058303

65 1 0 -2.512421 5.364975 -0.058303

66 1 0 2.487843 -7.828541 -0.258814

67 1 0 1.243262 -9.951788 -0.435088

68 1 0 -1.243262 -9.951788 -0.435088

69 1 0 -2.487843 -7.828541 -0.258814

70 1 0 7.828556 -2.487843 -0.258655

71 1 0 9.951808 -1.243262 -0.434870

72 1 0 9.951808 1.243262 -0.434870

73 1 0 7.828556 2.487843 -0.258655

74 1 0 -2.487843 7.828541 -0.258814

75 1 0 -1.243262 9.951788 -0.435088

76 1 0 1.243262 9.951788 -0.435088

77 1 0 2.487843 7.828541 -0.258814

78 1 0 -7.828556 -2.487843 -0.258655

79 1 0 -9.951808 -1.243262 -0.434870

80 1 0 -9.951808 1.243262 -0.434870

81 1 0 -7.828556 2.487843 -0.258655

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

Rotational constants (GHZ): 0.0383619 0.0383618 0.0192836

Leave Link 202 at Thu Sep 19 00:35:28 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: 58 59 60 61 62 63 64 65 66 67

Centers: 68 69 70 71 72 73 74 75 76 77

Centers: 78 79 80 81 1 3 4 5 7 9

Centers: 10 11 13 14 15 17 20 21 22 23

Centers: 26 27 28 29 30 31 32 33 34 35

Centers: 36 37 38 39 40 41 42 43 44 45

Centers: 46 47 48 49 50 51 52 53 54 55

Centers: 56 57 2 6 8 12 16 18 19 24

6-311G\*

\*\*\*\*

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

Pseudopotential Parameters

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

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

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

1 6

No pseudopotential on this center.

2 7

No pseudopotential on this center.

3 6

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 7

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 7

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 7

No pseudopotential on this center.

17 6

No pseudopotential on this center.

18 7

No pseudopotential on this center.

19 7

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 6

No pseudopotential on this center.

24 7

No pseudopotential on this center.

25 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

26 6

No pseudopotential on this center.

27 6

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78 1

No pseudopotential on this center.

79 1

No pseudopotential on this center.

80 1

No pseudopotential on this center.

81 1

No pseudopotential on this center.

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

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

There are 307 symmetry adapted cartesian basis functions of A1 symmetry.

There are 278 symmetry adapted cartesian basis functions of A2 symmetry.

There are 289 symmetry adapted cartesian basis functions of B1 symmetry.

There are 289 symmetry adapted cartesian basis functions of B2 symmetry.

There are 289 symmetry adapted basis functions of A1 symmetry.

There are 265 symmetry adapted basis functions of A2 symmetry.

There are 275 symmetry adapted basis functions of B1 symmetry.

There are 275 symmetry adapted basis functions of B2 symmetry.

1104 basis functions, 1951 primitive gaussians, 1163 cartesian basis functions

190 alpha electrons 190 beta electrons

nuclear repulsion energy 6888.8260724835 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= 81 NActive= 81 NUniq= 22 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= -0.2360382768 Hartrees.

Nuclear repulsion after empirical dispersion term = 6888.5900342067 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= 81.

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 = 81

GePol: Total number of spheres = 81

GePol: Number of exposed spheres = 81 (100.00%)

GePol: Number of points = 6354

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.19D-08

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 244

GePol: Fraction of low-weight points (<1% of avg) = 3.84%

GePol: Cavity surface area = 671.282 Ang\*\*2

GePol: Cavity volume = 693.864 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0172173388 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 6888.5728168679 Hartrees.

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

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 64980 NPrTT= 323086 LenC2= 36709 LenP2D= 95142.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 1104 RedAO= T EigKep= 2.88D-05 NBF= 289 265 275 275

NBsUse= 1104 1.00D-06 EigRej= -1.00D+00 NBFU= 289 265 275 275

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= 1060 1060 1060 1060 1060 MxSgAt= 81 MxSgA2= 81.

Leave Link 302 at Thu Sep 19 00:35:30 2019, MaxMem= 1342177280 cpu: 13.9

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

Leave Link 308 at Thu Sep 19 00:35:30 2019, MaxMem= 1342177280 cpu: 2.6

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

DipDrv: MaxL=1.

Leave Link 303 at Thu Sep 19 00:35:30 2019, MaxMem= 1342177280 cpu: 1.6

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

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

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

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

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 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= -2348.40225961047

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

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

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

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

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

Leave Link 401 at Thu Sep 19 00:35:34 2019, MaxMem= 1342177280 cpu: 33.9

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 4099732 IEndB= 4099732 NGot= 1342177280 MDV= 1339447921

LenX= 1339447921 LenY= 1338094189

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= 420000000 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 1.18D-14 for 6350.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.94D-15 for 6344 5465.

Iteration 1 A^-1\*A deviation from unit magnitude is 1.13D-14 for 6350.

Iteration 1 A^-1\*A deviation from orthogonality is 4.32D-09 for 2962 2960.

Iteration 2 A\*A^-1 deviation from unit magnitude is 2.44D-15 for 56.

Iteration 2 A\*A^-1 deviation from orthogonality is 3.67D-15 for 2903 323.

Iteration 2 A^-1\*A deviation from unit magnitude is 9.99D-16 for 2869.

Iteration 2 A^-1\*A deviation from orthogonality is 3.63D-16 for 4661 4616.

E= -2347.08035811961

DIIS: error= 8.83D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -2347.08035811961 IErMin= 1 ErrMin= 8.83D-02

ErrMax= 8.83D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.37D+00 BMatP= 1.37D+00

IDIUse=3 WtCom= 1.17D-01 WtEn= 8.83D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.095 Goal= None Shift= 0.000

GapD= 0.095 DampG=0.500 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.16D-03 MaxDP=8.86D-02 OVMax= 1.93D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.70D-04 CP: 9.98D-01

E= -2347.30172924527 Delta-E= -0.221371125661 Rises=F Damp=T

DIIS: error= 6.32D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -2347.30172924527 IErMin= 2 ErrMin= 6.32D-02

ErrMax= 6.32D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.10D-01 BMatP= 1.37D+00

IDIUse=3 WtCom= 3.68D-01 WtEn= 6.32D-01

Coeff-Com: -0.303D+01 0.403D+01

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

Coeff: -0.111D+01 0.211D+01

Gap= 0.073 Goal= None Shift= 0.000

RMSDP=1.30D-03 MaxDP=5.68D-02 DE=-2.21D-01 OVMax= 7.81D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.89D-04 CP: 9.81D-01 3.00D+00

E= -2347.98333086242 Delta-E= -0.681601617152 Rises=F Damp=F

DIIS: error= 4.02D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -2347.98333086242 IErMin= 3 ErrMin= 4.02D-02

ErrMax= 4.02D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.17D-01 BMatP= 8.10D-01

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

Coeff-Com: 0.196D+01-0.204D+01 0.108D+01

Coeff-En: 0.265D-01 0.000D+00 0.974D+00

Coeff: 0.118D+01-0.122D+01 0.103D+01

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=6.42D-04 MaxDP=2.78D-02 DE=-6.82D-01 OVMax= 5.31D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 3.73D-04 CP: 9.83D-01 3.00D+00 3.38D-01

E= -2348.13271975824 Delta-E= -0.149388895821 Rises=F Damp=F

DIIS: error= 1.59D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -2348.13271975824 IErMin= 4 ErrMin= 1.59D-02

ErrMax= 1.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.90D-02 BMatP= 2.17D-01

IDIUse=3 WtCom= 8.41D-01 WtEn= 1.59D-01

Coeff-Com: -0.217D+00 0.282D+00 0.263D+00 0.672D+00

Coeff-En: 0.000D+00 0.000D+00 0.889D-01 0.911D+00

Coeff: -0.183D+00 0.237D+00 0.235D+00 0.710D+00

Gap= 0.070 Goal= None Shift= 0.000

RMSDP=1.84D-04 MaxDP=9.58D-03 DE=-1.49D-01 OVMax= 2.28D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 4.81D-05 CP: 9.83D-01 3.00D+00 5.17D-01 7.12D-01

E= -2348.16291566022 Delta-E= -0.030195901973 Rises=F Damp=F

DIIS: error= 1.64D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -2348.16291566022 IErMin= 5 ErrMin= 1.64D-03

ErrMax= 1.64D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-03 BMatP= 3.90D-02

IDIUse=3 WtCom= 9.84D-01 WtEn= 1.64D-02

Coeff-Com: -0.173D+00 0.203D+00 0.100D+00 0.419D+00 0.451D+00

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

Coeff: -0.170D+00 0.200D+00 0.984D-01 0.412D+00 0.460D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=2.97D-05 MaxDP=2.47D-03 DE=-3.02D-02 OVMax= 5.34D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.60D-05 CP: 9.83D-01 3.00D+00 5.03D-01 7.40D-01 5.85D-01

E= -2348.16448453667 Delta-E= -0.001568876454 Rises=F Damp=F

DIIS: error= 3.94D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -2348.16448453667 IErMin= 6 ErrMin= 3.94D-04

ErrMax= 3.94D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.69D-05 BMatP= 1.88D-03

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.94D-03

Coeff-Com: -0.953D-01 0.110D+00 0.281D-01 0.170D+00 0.234D+00 0.554D+00

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

Coeff: -0.949D-01 0.109D+00 0.280D-01 0.169D+00 0.233D+00 0.556D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=8.44D-06 MaxDP=6.06D-04 DE=-1.57D-03 OVMax= 1.70D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 4.99D-06 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.03D-01

CP: 5.96D-01

E= -2348.16452705325 Delta-E= -0.000042516576 Rises=F Damp=F

DIIS: error= 1.30D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -2348.16452705325 IErMin= 7 ErrMin= 1.30D-04

ErrMax= 1.30D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.72D-06 BMatP= 5.69D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.30D-03

Coeff-Com: -0.452D-01 0.516D-01 0.794D-02 0.653D-01 0.942D-01 0.342D+00

Coeff-Com: 0.484D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.116D+00

Coeff-En: 0.884D+00

Coeff: -0.451D-01 0.515D-01 0.793D-02 0.652D-01 0.941D-01 0.342D+00

Coeff: 0.484D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=2.53D-06 MaxDP=1.76D-04 DE=-4.25D-05 OVMax= 4.98D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.58D-06 CP: 9.83D-01 3.00D+00 5.06D-01 7.43D-01 6.07D-01

CP: 6.72D-01 6.96D-01

E= -2348.16453509518 Delta-E= -0.000008041932 Rises=F Damp=F

DIIS: error= 1.67D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -2348.16453509518 IErMin= 8 ErrMin= 1.67D-05

ErrMax= 1.67D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.20D-07 BMatP= 8.72D-06

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

Coeff-Com: -0.977D-02 0.111D-01 0.849D-03 0.110D-01 0.143D-01 0.988D-01

Coeff-Com: 0.202D+00 0.672D+00

Coeff: -0.977D-02 0.111D-01 0.849D-03 0.110D-01 0.143D-01 0.988D-01

Coeff: 0.202D+00 0.672D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=9.77D-07 MaxDP=4.33D-05 DE=-8.04D-06 OVMax= 1.37D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 7.71D-07 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.10D-01

CP: 6.90D-01 7.35D-01 9.62D-01

E= -2348.16453531474 Delta-E= -0.000000219559 Rises=F Damp=F

DIIS: error= 1.42D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -2348.16453531474 IErMin= 9 ErrMin= 1.42D-05

ErrMax= 1.42D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.79D-08 BMatP= 3.20D-07

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

Coeff-Com: 0.548D-03-0.696D-03-0.552D-03-0.248D-02-0.480D-02 0.128D-01

Coeff-Com: 0.503D-01 0.408D+00 0.537D+00

Coeff: 0.548D-03-0.696D-03-0.552D-03-0.248D-02-0.480D-02 0.128D-01

Coeff: 0.503D-01 0.408D+00 0.537D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=4.43D-07 MaxDP=2.22D-05 DE=-2.20D-07 OVMax= 9.35D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.74D-07 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.09D-01

CP: 6.89D-01 7.39D-01 9.75D-01 5.71D-01

E= -2348.16453540874 Delta-E= -0.000000093998 Rises=F Damp=F

DIIS: error= 2.50D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -2348.16453540874 IErMin=10 ErrMin= 2.50D-06

ErrMax= 2.50D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.74D-09 BMatP= 9.79D-08

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

Coeff-Com: 0.743D-03-0.874D-03-0.184D-03-0.129D-02-0.217D-02 0.174D-02

Coeff-Com: 0.999D-02 0.118D+00 0.211D+00 0.664D+00

Coeff: 0.743D-03-0.874D-03-0.184D-03-0.129D-02-0.217D-02 0.174D-02

Coeff: 0.999D-02 0.118D+00 0.211D+00 0.664D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=7.26D-08 MaxDP=2.74D-06 DE=-9.40D-08 OVMax= 1.27D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.29D-08 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.09D-01

CP: 6.90D-01 7.36D-01 9.75D-01 6.04D-01 1.01D+00

E= -2348.16453541089 Delta-E= -0.000000002157 Rises=F Damp=F

DIIS: error= 1.23D-06 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -2348.16453541089 IErMin=11 ErrMin= 1.23D-06

ErrMax= 1.23D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.22D-10 BMatP= 2.74D-09

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

Coeff-Com: 0.306D-03-0.354D-03-0.263D-04-0.346D-03-0.503D-03-0.125D-03

Coeff-Com: -0.256D-04 0.141D-01 0.506D-01 0.382D+00 0.554D+00

Coeff: 0.306D-03-0.354D-03-0.263D-04-0.346D-03-0.503D-03-0.125D-03

Coeff: -0.256D-04 0.141D-01 0.506D-01 0.382D+00 0.554D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=2.35D-08 MaxDP=1.37D-06 DE=-2.16D-09 OVMax= 6.21D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 1.55D-08 CP: 9.83D-01 3.00D+00 5.05D-01 7.44D-01 6.09D-01

CP: 6.90D-01 7.36D-01 9.75D-01 6.06D-01 1.04D+00

CP: 7.30D-01

E= -2348.16453541161 Delta-E= -0.000000000713 Rises=F Damp=F

DIIS: error= 2.54D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -2348.16453541161 IErMin=12 ErrMin= 2.54D-07

ErrMax= 2.54D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.40D-11 BMatP= 7.22D-10

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

Coeff-Com: -0.487D-05 0.662D-05-0.738D-06 0.889D-05 0.259D-04-0.142D-03

Coeff-Com: -0.473D-03-0.530D-02-0.459D-02 0.249D-01 0.135D+00 0.850D+00

Coeff: -0.487D-05 0.662D-05-0.738D-06 0.889D-05 0.259D-04-0.142D-03

Coeff: -0.473D-03-0.530D-02-0.459D-02 0.249D-01 0.135D+00 0.850D+00

Gap= 0.069 Goal= None Shift= 0.000

RMSDP=5.06D-09 MaxDP=2.91D-07 DE=-7.13D-10 OVMax= 2.38D-06

Error on total polarization charges = 0.08885

SCF Done: E(RB3LYP) = -2348.16453541 A.U. after 12 cycles

NFock= 12 Conv=0.51D-08 -V/T= 1.9830

KE= 2.388757903125D+03 PE=-1.931954529452D+04 EE= 7.694050039119D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -10.80

(included in total energy above)

Leave Link 502 at Thu Sep 19 00:40:06 2019, MaxMem= 1342177280 cpu: 2417.0

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

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

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

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

ICtDFT= 12500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

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

Largest core mixing into a valence orbital is 2.24D-05

Range of M.O.s used for correlation: 57 1104

NBasis= 1104 NAE= 190 NBE= 190 NFC= 56 NFV= 0

NROrb= 1048 NOA= 134 NOB= 134 NVA= 914 NVB= 914

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.15994799D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.69234720D-01

Leave Link 801 at Thu Sep 19 00:40:06 2019, MaxMem= 1342177280 cpu: 3.9

(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 231192000000 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 7.33D-15 for 6348.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.02D-15 for 4265 379.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.55D-15 for 6348.

Iteration 1 A^-1\*A deviation from orthogonality is 3.13D-15 for 6335 6248.

Making orbital integer symmetry assigments:

Orbital symmetries:

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

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

40 initial guesses have been made.

Convergence on wavefunction: 0.001000000000000

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

Max sub-space: 200 roots to seek: 40 dimension of matrix: 244952

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 7 was old state 10

New state 8 was old state 7

New state 9 was old state 8

New state 10 was old state 9

Excitation Energies [eV] at current iteration:

Root 1 : 1.943051546683700

Root 2 : 1.943055320519200

Root 3 : 2.736598400401995

Root 4 : 2.772943270884025

Root 5 : 2.867223450914185

Root 6 : 2.867225370550662

Root 7 : 2.991796752107804

Root 8 : 3.055239833564313

Root 9 : 3.055245148774546

Root 10 : 3.056556117199539

Root 11 : 3.104471657304943

Root 12 : 3.247907863832520

Root 13 : 3.304933937768626

Root 14 : 3.491693863444175

Root 15 : 3.491699577243956

Root 16 : 3.527361860761860

Root 17 : 3.553659270509933

Root 18 : 3.617180360676686

Root 19 : 3.617181517526131

Root 20 : 3.666595002635897

Root 21 : 3.666601977120606

Root 22 : 3.700397585098805

Root 23 : 3.703969086296245

Root 24 : 3.703974113449681

Root 25 : 3.736489734107086

Root 26 : 3.736496294571364

Root 27 : 3.754790435636865

Root 28 : 4.215469423501908

Root 29 : 4.215471274786450

Root 30 : 4.281019398764232

Root 31 : 4.355113040810998

Root 32 : 4.355113383692190

Root 33 : 4.389230804297181

Root 34 : 4.457617634344838

Root 35 : 4.515027889178764

Root 36 : 4.515030817714573

Root 37 : 4.640211500441041

Root 38 : 4.824650613895065

Root 39 : 4.824650772552491

Root 40 : 4.848061906815394

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 0.066080023930176

Root 2 not converged, maximum delta is 0.066079727307505

Root 3 not converged, maximum delta is 0.129873438619475

Root 4 not converged, maximum delta is 0.158219266232764

Root 5 not converged, maximum delta is 0.160903960049107

Root 6 not converged, maximum delta is 0.160901474502347

Root 7 not converged, maximum delta is 0.163467617984334

Root 8 not converged, maximum delta is 0.147394711864075

Root 9 not converged, maximum delta is 0.147391959594933

Root 10 not converged, maximum delta is 0.024266740533376

Excitation Energies [eV] at current iteration:

Root 1 : 1.714804414040503 Change is -0.228247132643197

Root 2 : 1.714808528695980 Change is -0.228246791823220

Root 3 : 2.604237121644787 Change is -0.132361278757208

Root 4 : 2.680085399542716 Change is -0.092857871341309

Root 5 : 2.792529374941301 Change is -0.074694075972884

Root 6 : 2.792530431758894 Change is -0.074694938791768

Root 7 : 2.928339101348816 Change is -0.063457650758988

Root 8 : 2.951247620601564 Change is -0.103992212962750

Root 9 : 2.951253416499021 Change is -0.103991732275525

Root 10 : 2.960735456301635 Change is -0.095820660897905

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 0.017222359775264

Root 2 not converged, maximum delta is 0.017222364992204

Root 3 not converged, maximum delta is 0.015420478438914

Root 4 not converged, maximum delta is 0.014715445203377

Root 5 not converged, maximum delta is 0.013251843379326

Root 6 not converged, maximum delta is 0.013251571731948

Root 7 not converged, maximum delta is 0.018850723136580

Root 8 not converged, maximum delta is 0.012738652614395

Root 9 not converged, maximum delta is 0.012738347198479

Root 10 not converged, maximum delta is 0.064464343196782

Excitation Energies [eV] at current iteration:

Root 1 : 1.699293194192441 Change is -0.015511219848062

Root 2 : 1.699297365655489 Change is -0.015511163040491

Root 3 : 2.595276090303587 Change is -0.008961031341200

Root 4 : 2.674553765688627 Change is -0.005531633854089

Root 5 : 2.784663141806842 Change is -0.007866233134459

Root 6 : 2.784664117139980 Change is -0.007866314618914

Root 7 : 2.925091455350907 Change is -0.003247645997909

Root 8 : 2.943631872837604 Change is -0.007615747763960

Root 9 : 2.943637656479526 Change is -0.007615760019495

Root 10 : 2.950108028111722 Change is -0.010627428189913

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 0.003267466085234

Root 2 not converged, maximum delta is 0.003267432286005

Root 3 not converged, maximum delta is 0.002745291546361

Root 4 not converged, maximum delta is 0.001960189738076

Root 5 not converged, maximum delta is 0.003092799698849

Root 6 not converged, maximum delta is 0.003092847835402

Root 7 not converged, maximum delta is 0.002104616316496

Root 8 not converged, maximum delta is 0.004450137830676

Root 9 not converged, maximum delta is 0.004450167111436

Root 10 not converged, maximum delta is 0.031286557939196

Excitation Energies [eV] at current iteration:

Root 1 : 1.697430121526239 Change is -0.001863072666202

Root 2 : 1.697434298988322 Change is -0.001863066667167

Root 3 : 2.594453220741411 Change is -0.000822869562176

Root 4 : 2.673889746396525 Change is -0.000664019292102

Root 5 : 2.783779198966307 Change is -0.000883942840535

Root 6 : 2.783780163670490 Change is -0.000883953469490

Root 7 : 2.924695192845736 Change is -0.000396262505172

Root 8 : 2.942497937793928 Change is -0.001133935043676

Root 9 : 2.942503719180477 Change is -0.001133937299048

Root 10 : 2.948164526612305 Change is -0.001943501499418

Iteration 5 Dimension 120 NMult 100 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 not converged, maximum delta is 0.001012220318404

Root 2 not converged, maximum delta is 0.001012220134025

Root 3 has converged.

Root 4 has converged.

Root 5 has converged.

Root 6 has converged.

Root 7 not converged, maximum delta is 0.001041565979628

Root 8 has converged.

Root 9 has converged.

Root 10 not converged, maximum delta is 0.006205087158221

Excitation Energies [eV] at current iteration:

Root 1 : 1.697273075160572 Change is -0.000157046365667

Root 2 : 1.697277252019953 Change is -0.000157046968369

Root 3 : 2.594346103236862 Change is -0.000107117504549

Root 4 : 2.673821590020446 Change is -0.000068156376079

Root 5 : 2.783647432501460 Change is -0.000131766464847

Root 6 : 2.783648395977138 Change is -0.000131767693353

Root 7 : 2.924650212847788 Change is -0.000044979997948

Root 8 : 2.942376135791093 Change is -0.000121802002835

Root 9 : 2.942381917937528 Change is -0.000121801242949

Root 10 : 2.947851391327532 Change is -0.000313135284772

Iteration 6 Dimension 128 NMult 120 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 not converged, maximum delta is 0.002182743731251

Excitation Energies [eV] at current iteration:

Root 1 : 1.697264113629540 Change is -0.000008961531032

Root 2 : 1.697268290518676 Change is -0.000008961501277

Root 3 : 2.594345864507389 Change is -0.000000238729473

Root 4 : 2.673818728898377 Change is -0.000002861122069

Root 5 : 2.783647289609131 Change is -0.000000142892329

Root 6 : 2.783648253154466 Change is -0.000000142822672

Root 7 : 2.924647035409499 Change is -0.000003177438288

Root 8 : 2.942374013358126 Change is -0.000002122432967

Root 9 : 2.942379795485822 Change is -0.000002122451706

Root 10 : 2.947779455231056 Change is -0.000071936096477

Iteration 7 Dimension 130 NMult 128 NNew 2

CISAX will form 2 AO SS matrices at one time.

NMat= 2 NSing= 2 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 has converged.

Root 4 has converged.

Root 5 has converged.

Root 6 has converged.

Root 7 has converged.

Root 8 has converged.

Root 9 has converged.

Root 10 not converged, maximum delta is 0.001175435727393

Excitation Energies [eV] at current iteration:

Root 1 : 1.697264113629685 Change is 0.000000000000145

Root 2 : 1.697268290518676 Change is 0.000000000000000

Root 3 : 2.594345864507357 Change is -0.000000000000032

Root 4 : 2.673818728898500 Change is 0.000000000000123

Root 5 : 2.783647289609013 Change is -0.000000000000118

Root 6 : 2.783648253154407 Change is -0.000000000000059

Root 7 : 2.924647035409527 Change is 0.000000000000028

Root 8 : 2.942374013358070 Change is -0.000000000000056

Root 9 : 2.942379795485849 Change is 0.000000000000028

Root 10 : 2.947771061565974 Change is -0.000008393665081

Convergence on energies, max DE= 8.39D-06.

Convergence on expansion vectors.

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

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

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

1PDM for each excited state written to RWF 633

Ground to excited state transition densities written to RWF 633

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

state X Y Z Dip. S. Osc.

1 0.0000 4.5574 -0.0000 20.7701 0.8637

2 4.5574 -0.0000 0.0000 20.7700 0.8637

3 0.0000 -0.0000 0.0000 0.0000 0.0000

4 0.0000 -0.0000 -0.0000 0.0000 0.0000

5 0.0000 0.7786 0.0000 0.6062 0.0413

6 0.7786 -0.0000 0.0000 0.6062 0.0413

7 -0.0000 -0.0000 -0.0000 0.0000 0.0000

8 0.0000 -2.1345 -0.0000 4.5563 0.3284

9 2.1345 0.0000 0.0000 4.5563 0.3284

10 0.0000 0.0000 -0.0001 0.0000 0.0000

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

state X Y Z Dip. S. Osc.

1 -0.0000 -0.2851 -0.0000 0.0813 0.8690

2 -0.2851 0.0000 -0.0000 0.0813 0.8690

3 -0.0000 -0.0000 0.0000 0.0000 0.0000

4 -0.0000 0.0000 -0.0000 0.0000 0.0000

5 -0.0000 -0.0709 -0.0000 0.0050 0.0327

6 -0.0709 0.0000 -0.0000 0.0050 0.0327

7 0.0000 0.0000 0.0000 0.0000 0.0000

8 -0.0000 0.2243 0.0000 0.0503 0.3101

9 -0.2243 -0.0000 0.0000 0.0503 0.3101

10 -0.0000 -0.0000 0.0000 0.0000 0.0000

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

state X Y Z

1 0.1347 -0.0000 -0.0000

2 -0.0000 -0.1347 -0.0000

3 0.0000 -0.0000 0.0002

4 -0.0000 0.0000 0.6281

5 0.0934 -0.0000 0.0000

6 -0.0000 -0.0934 -0.0000

7 -0.0000 0.0000 1.0221

8 -0.1395 -0.0000 -0.0000

9 0.0000 -0.1395 0.0000

10 0.0000 -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 0.0746

2 -0.0000 0.0000 -0.0000 0.0000 0.0746 -0.0000

3 0.0000 -0.0000 0.0000 0.8095 0.0000 0.0000

4 0.0000 0.0000 0.0000 -0.0004 0.0000 0.0000

5 0.0000 0.0000 0.0000 0.0000 0.0000 0.0355

6 0.0000 0.0000 -0.0000 -0.0000 0.0355 -0.0000

7 0.0000 -0.0000 0.0000 -0.0002 -0.0000 -0.0000

8 0.0000 -0.0000 -0.0000 -0.0000 0.0000 -0.1337

9 -0.0000 0.0000 -0.0000 -0.0000 0.1336 0.0000

10 2.7241 -2.7245 0.0000 -0.0000 0.0000 0.0000

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

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

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

1 0.0000 -0.0000 0.0000 -0.0000 90.00

2 -0.0000 0.0000 -0.0000 0.0000 90.00

3 0.0000 -0.0000 0.0000 0.0000 90.00

4 -0.0000 -0.0000 0.0000 -0.0000 90.00

5 0.0000 -0.0000 0.0000 0.0000 90.00

6 -0.0000 0.0000 -0.0000 -0.0000 90.00

7 0.0000 0.0000 -0.0000 0.0000 90.00

8 -0.0000 0.0000 -0.0000 0.0000 90.00

9 0.0000 -0.0000 0.0000 -0.0000 90.00

10 -0.0000 0.0000 -0.0000 -0.0000 90.00

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

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

state XX YY ZZ R(length)

1 -0.0000 0.0000 -0.0000 -0.0000

2 0.0000 -0.0000 0.0000 0.0000

3 -0.0000 -0.0000 -0.0000 -0.0000

4 0.0000 0.0000 0.0000 0.0000

5 -0.0000 0.0000 -0.0000 0.0000

6 0.0000 -0.0000 0.0000 -0.0000

7 -0.0000 0.0000 0.0000 0.0000

8 0.0000 -0.0000 -0.0000 0.0000

9 -0.0000 0.0000 -0.0000 -0.0000

10 -0.0000 0.0000 -0.0000 -0.0000

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

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

1 -0.0000 -1.2995 0.0000 1.2995 0.8663

2 -1.2995 -0.0000 -0.0000 1.2995 0.8663

3 -0.0000 0.0000 0.0000 0.0000 0.0000

4 -0.0000 -0.0000 0.0000 0.0000 0.0000

5 -0.0000 -0.0552 -0.0000 0.0552 0.0368

6 -0.0552 -0.0000 -0.0000 0.0552 0.0368

7 -0.0000 -0.0000 -0.0000 0.0000 0.0000

8 -0.0000 -0.4787 -0.0000 0.4787 0.3191

9 -0.4787 -0.0000 0.0000 0.4787 0.3191

10 -0.0000 -0.0000 -0.0000 0.0000 0.0000

Excitation energies and oscillator strengths:

Excited State 1: Singlet-B2 1.6973 eV 730.49 nm f=0.8637 <S\*\*2>=0.000

63 -> 282 -0.00120

68 -> 261 0.00101

77 -> 245 -0.00105

87 -> 252 0.00164

93 -> 254 0.00113

93 -> 261 0.00146

94 -> 252 0.00125

96 -> 257 -0.00106

96 -> 265 -0.00102

99 -> 225 -0.00104

101 -> 265 0.00196

101 -> 277 -0.00126

101 -> 345 -0.00123

106 -> 257 0.00103

107 -> 243 -0.00133

107 -> 252 0.00246

107 -> 266 -0.00188

107 -> 275 -0.00143

108 -> 242 -0.00232

108 -> 251 -0.00105

108 -> 256 -0.00159

108 -> 260 -0.00107

108 -> 290 -0.00187

108 -> 361 -0.00201

108 -> 393 0.00163

109 -> 254 -0.00120

110 -> 290 -0.00152

111 -> 238 0.00131

111 -> 243 -0.00131

111 -> 250 0.00144

112 -> 253 -0.00146

112 -> 273 0.00113

112 -> 386 0.00101

113 -> 210 -0.00116

113 -> 213 -0.00139

113 -> 215 0.00101

113 -> 250 0.00129

115 -> 261 0.00138

116 -> 212 -0.00154

117 -> 208 -0.00148

117 -> 239 -0.00166

117 -> 245 -0.00284

117 -> 257 -0.00229

117 -> 265 -0.00196

117 -> 277 0.00114

117 -> 291 -0.00100

117 -> 345 -0.00116

117 -> 404 0.00103

118 -> 212 0.00138

118 -> 222 -0.00123

118 -> 236 -0.00115

119 -> 242 0.00130

119 -> 282 0.00116

120 -> 218 -0.00245

120 -> 243 0.00106

120 -> 250 0.00190

121 -> 208 0.00127

121 -> 245 0.00273

121 -> 253 -0.00135

121 -> 262 -0.00210

121 -> 345 0.00108

122 -> 196 0.00223

122 -> 203 0.00133

122 -> 221 0.00281

122 -> 234 -0.00282

122 -> 295 -0.00155

123 -> 217 0.00219

123 -> 235 -0.00110

123 -> 253 -0.00109

124 -> 214 0.00288

124 -> 219 0.00222

124 -> 230 0.00164

125 -> 250 -0.00114

126 -> 208 -0.00136

126 -> 217 -0.00264

126 -> 228 0.00121

127 -> 254 -0.00149

128 -> 193 0.00121

128 -> 194 -0.00108

128 -> 201 -0.00160

128 -> 205 -0.00130

128 -> 207 0.00129

128 -> 250 0.00143

129 -> 197 0.00142

129 -> 206 0.00135

129 -> 214 -0.00137

129 -> 251 0.00103

130 -> 197 -0.00283

130 -> 206 -0.00274

130 -> 231 -0.00175

131 -> 193 0.00242

131 -> 194 -0.00207

131 -> 201 -0.00260

131 -> 202 -0.00195

131 -> 205 -0.00163

131 -> 207 0.00253

131 -> 215 0.00164

131 -> 229 0.00183

131 -> 232 0.00170

131 -> 317 0.00105

131 -> 344 0.00118

132 -> 217 -0.00132

132 -> 239 -0.00210

132 -> 253 -0.00125

133 -> 212 0.00195

133 -> 244 0.00115

134 -> 244 -0.00107

134 -> 258 0.00147

134 -> 261 -0.00178

135 -> 210 -0.00168

135 -> 213 -0.00192

135 -> 218 0.00146

135 -> 243 -0.00112

135 -> 259 0.00113

136 -> 242 0.00155

137 -> 212 -0.00189

137 -> 244 0.00122

138 -> 210 0.00148

138 -> 243 -0.00126

138 -> 250 -0.00276

138 -> 259 0.00115

138 -> 271 0.00126

138 -> 279 -0.00108

139 -> 214 0.00117

139 -> 224 -0.00105

139 -> 237 -0.00161

139 -> 241 0.00167

139 -> 282 -0.00140

140 -> 223 -0.00156

140 -> 228 0.00135

140 -> 253 0.00154

140 -> 265 0.00149

141 -> 192 -0.00738

141 -> 199 -0.00214

141 -> 221 0.00121

141 -> 295 -0.00153

142 -> 223 -0.00157

142 -> 228 0.00108

142 -> 239 -0.00124

142 -> 253 0.00118

143 -> 219 0.00149

143 -> 224 0.00231

143 -> 230 -0.00130

143 -> 241 -0.00115

143 -> 303 0.00112

144 -> 210 0.00116

144 -> 250 -0.00204

144 -> 259 0.00130

145 -> 228 -0.00146

145 -> 239 0.00110

145 -> 253 0.00295

145 -> 262 0.00138

145 -> 265 0.00288

146 -> 234 0.00129

146 -> 300 0.00131

147 -> 206 -0.00117

147 -> 231 -0.00118

148 -> 193 0.00187

148 -> 205 -0.00175

148 -> 207 0.00196

148 -> 229 0.00104

148 -> 298 -0.00143

148 -> 299 -0.00139

150 -> 191 0.00703

150 -> 195 -0.00102

150 -> 200 0.00279

150 -> 233 -0.00183

150 -> 296 0.00125

151 -> 192 -0.00806

151 -> 199 -0.00157

151 -> 203 -0.00121

151 -> 221 0.00149

151 -> 300 -0.00126

152 -> 212 -0.00156

152 -> 236 -0.00157

152 -> 240 0.00191

152 -> 254 0.00145

152 -> 264 0.00117

153 -> 263 0.00122

153 -> 272 -0.00113

153 -> 282 0.00235

154 -> 205 -0.00144

154 -> 210 -0.00167

154 -> 213 -0.00121

154 -> 215 -0.00146

154 -> 238 -0.00278

154 -> 243 -0.00253

154 -> 279 -0.00105

155 -> 212 0.00104

155 -> 236 0.00169

155 -> 244 0.00123

155 -> 258 -0.00102

155 -> 261 0.00208

155 -> 274 -0.00110

155 -> 292 -0.00105

155 -> 318 0.00119

156 -> 228 0.00136

156 -> 253 -0.00193

157 -> 243 0.00105

157 -> 250 0.00225

157 -> 259 -0.00175

157 -> 278 0.00118

157 -> 285 0.00102

158 -> 219 0.00101

158 -> 224 0.00126

158 -> 230 -0.00148

158 -> 237 -0.00138

158 -> 241 0.00129

158 -> 269 0.00137

158 -> 282 0.00110

159 -> 223 -0.00102

159 -> 235 0.00108

159 -> 239 0.00164

159 -> 253 0.00208

159 -> 257 0.00121

159 -> 265 0.00207

160 -> 197 -0.00456

160 -> 198 0.00114

160 -> 226 0.00101

160 -> 315 -0.00160

161 -> 193 0.00345

161 -> 194 0.00368

161 -> 202 -0.00262

161 -> 207 0.00172

161 -> 314 -0.00144

162 -> 214 0.00100

162 -> 242 -0.00116

162 -> 282 0.00141

162 -> 290 -0.00134

163 -> 201 0.00204

163 -> 205 0.00273

163 -> 210 0.00203

163 -> 215 0.00302

163 -> 225 -0.00281

163 -> 229 -0.00139

163 -> 232 0.00175

163 -> 243 0.00282

163 -> 266 -0.00133

164 -> 212 -0.00103

164 -> 222 -0.00235

164 -> 227 -0.00242

165 -> 209 -0.00172

165 -> 212 0.00123

165 -> 216 0.00189

165 -> 222 0.00220

165 -> 227 0.00135

165 -> 261 0.00181

165 -> 264 0.00110

165 -> 283 -0.00104

166 -> 192 -0.00739

166 -> 196 -0.00156

166 -> 234 -0.00164

167 -> 198 0.00128

167 -> 206 -0.00120

167 -> 214 -0.00106

167 -> 242 -0.00352

167 -> 256 -0.00174

167 -> 263 -0.00134

167 -> 272 0.00119

167 -> 282 -0.00111

167 -> 290 -0.00257

167 -> 306 -0.00101

167 -> 361 0.00124

168 -> 193 0.00120

168 -> 194 0.00166

168 -> 201 0.00355

168 -> 205 0.00428

168 -> 213 -0.00119

168 -> 215 0.00397

168 -> 218 -0.00271

168 -> 225 0.00205

168 -> 238 -0.00156

168 -> 243 0.00327

168 -> 252 -0.00225

168 -> 259 0.00136

168 -> 266 -0.00117

168 -> 271 0.00238

168 -> 275 -0.00152

168 -> 285 -0.00127

168 -> 287 0.00112

169 -> 192 -0.00847

169 -> 196 0.00110

169 -> 199 -0.00482

169 -> 203 -0.00128

169 -> 221 0.00246

169 -> 248 0.00104

169 -> 324 -0.00121

170 -> 193 -0.00195

170 -> 194 -0.00639

170 -> 201 -0.00350

170 -> 202 0.00116

170 -> 207 0.00281

170 -> 215 0.00226

170 -> 229 0.00113

170 -> 232 0.00115

170 -> 255 -0.00191

170 -> 317 -0.00101

170 -> 347 -0.00107

171 -> 197 -0.00104

171 -> 198 0.00417

171 -> 206 -0.00317

171 -> 226 0.00185

171 -> 231 -0.00205

171 -> 247 0.00188

171 -> 315 -0.00159

172 -> 209 -0.00113

172 -> 240 0.00107

172 -> 244 -0.00284

172 -> 254 -0.00117

172 -> 261 -0.00215

172 -> 264 0.00110

172 -> 295 -0.00112

173 -> 191 0.00695

173 -> 195 0.00559

173 -> 204 0.00467

173 -> 249 0.00140

173 -> 321 -0.00201

174 -> 191 0.00418

174 -> 195 0.00199

174 -> 204 0.00375

174 -> 220 -0.00338

174 -> 249 -0.00149

174 -> 321 0.00131

174 -> 325 -0.00121

175 -> 193 0.00189

175 -> 194 0.00151

175 -> 205 0.00345

175 -> 207 0.00534

175 -> 229 -0.00145

175 -> 232 -0.00128

176 -> 197 0.00647

176 -> 198 -0.00296

176 -> 206 0.00476

176 -> 226 -0.00263

176 -> 246 0.00230

176 -> 322 -0.00119

176 -> 335 0.00164

177 -> 201 -0.00208

177 -> 205 -0.00285

177 -> 207 0.00118

177 -> 215 -0.00340

177 -> 218 0.00179

177 -> 238 -0.00242

177 -> 250 -0.00202

177 -> 252 -0.00673

177 -> 259 0.00129

177 -> 266 0.00122

177 -> 275 0.00133

177 -> 278 -0.00126

177 -> 285 -0.00125

177 -> 287 -0.00100

177 -> 297 0.00101

177 -> 302 -0.00159

178 -> 237 0.00129

178 -> 242 0.00372

178 -> 251 -0.00198

178 -> 256 0.00170

178 -> 263 0.00117

178 -> 272 -0.00149

178 -> 290 0.00252

178 -> 303 -0.00121

178 -> 306 0.00104

178 -> 323 0.00110

179 -> 192 0.00117

179 -> 209 0.00255

179 -> 212 0.00133

179 -> 216 0.00208

179 -> 244 0.00523

179 -> 248 0.00119

179 -> 254 0.00265

179 -> 258 0.00413

179 -> 264 -0.00179

179 -> 268 -0.00139

179 -> 274 0.00273

179 -> 283 0.00195

179 -> 292 -0.00124

179 -> 304 -0.00116

179 -> 312 0.00166

179 -> 324 -0.00136

179 -> 385 0.00105

179 -> 398 0.00119

179 -> 403 0.00106

180 -> 191 -0.00163

180 -> 208 -0.00100

180 -> 223 0.00119

180 -> 235 0.00101

180 -> 239 -0.00279

180 -> 245 -0.00274

180 -> 249 0.00108

180 -> 262 0.00217

180 -> 265 -0.00411

180 -> 267 0.00113

180 -> 273 0.00170

180 -> 277 0.00143

180 -> 296 -0.00166

181 -> 192 0.07325

181 -> 196 0.00230

181 -> 199 0.01131

181 -> 203 0.00516

181 -> 221 -0.00294

181 -> 234 -0.00351

181 -> 248 -0.00192

182 -> 192 -0.07515

182 -> 196 -0.01268

182 -> 199 -0.00585

182 -> 203 -0.00114

182 -> 221 0.00112

183 -> 197 0.00908

183 -> 198 0.00575

183 -> 206 -0.00263

183 -> 226 0.00358

183 -> 231 -0.00388

183 -> 246 -0.00113

183 -> 247 0.00155

184 -> 193 -0.00416

184 -> 201 -0.00546

184 -> 202 -0.00309

184 -> 205 -0.00226

184 -> 207 0.00231

184 -> 215 0.00162

184 -> 229 0.00210

184 -> 232 0.00192

184 -> 255 -0.00168

184 -> 347 0.00105

185 -> 191 -0.01741

185 -> 195 -0.01202

185 -> 200 0.00486

185 -> 350 0.00203

186 -> 199 0.00887

186 -> 221 -0.00451

186 -> 222 -0.00102

186 -> 234 -0.00171

186 -> 248 -0.00142

186 -> 359 0.00105

187 -> 193 -0.00701

187 -> 194 0.00215

187 -> 202 0.00425

187 -> 205 -0.00284

187 -> 207 -0.01050

187 -> 229 0.00188

187 -> 232 0.00170

188 -> 197 -0.02774

188 -> 198 0.01427

188 -> 206 -0.00167

188 -> 226 0.00360

188 -> 354 0.00194

188 -> 364 -0.00168

189 -> 191 0.00669

189 -> 195 -0.00116

189 -> 200 0.01299

189 -> 204 0.00550

189 -> 220 -0.00515

189 -> 223 -0.00123

189 -> 350 0.00161

190 -> 191 0.70276

190 -> 195 -0.02340

190 -> 200 -0.00536

190 -> 204 -0.00471

190 -> 233 0.00257

190 -> 375 0.00190

190 -> 378 -0.00104

190 -> 390 -0.00131

190 -> 424 0.00112

63 <- 282 -0.00106

87 <- 252 0.00151

93 <- 254 0.00102

93 <- 261 0.00131

94 <- 252 0.00110

101 <- 265 0.00174

101 <- 277 -0.00115

101 <- 345 -0.00110

107 <- 243 -0.00115

107 <- 252 0.00220

107 <- 266 -0.00166

107 <- 275 -0.00127

108 <- 242 -0.00192

108 <- 256 -0.00129

108 <- 290 -0.00162

108 <- 361 -0.00179

108 <- 393 0.00145

110 <- 290 -0.00129

111 <- 238 0.00107

111 <- 243 -0.00110

111 <- 250 0.00115

112 <- 253 -0.00119

113 <- 213 -0.00108

113 <- 250 0.00107

115 <- 261 0.00116

116 <- 212 -0.00121

117 <- 208 -0.00118

117 <- 239 -0.00136

117 <- 245 -0.00238

117 <- 257 -0.00192

117 <- 265 -0.00168

117 <- 277 0.00101

117 <- 345 -0.00101

118 <- 212 0.00108

119 <- 242 0.00108

119 <- 282 0.00104

120 <- 218 -0.00195

120 <- 250 0.00160

121 <- 208 0.00104

121 <- 245 0.00227

121 <- 253 -0.00118

121 <- 262 -0.00184

122 <- 196 0.00161

122 <- 203 0.00100

122 <- 221 0.00226

122 <- 234 -0.00242

122 <- 295 -0.00137

123 <- 217 0.00167

124 <- 214 0.00219

124 <- 219 0.00170

124 <- 230 0.00128

126 <- 208 -0.00102

126 <- 217 -0.00202

127 <- 254 -0.00121

128 <- 201 -0.00119

128 <- 207 0.00106

128 <- 250 0.00114

129 <- 214 -0.00104

130 <- 197 -0.00176

130 <- 206 -0.00186

130 <- 231 -0.00129

131 <- 193 0.00168

131 <- 194 -0.00159

131 <- 201 -0.00195

131 <- 202 -0.00145

131 <- 205 -0.00120

131 <- 207 0.00206

131 <- 215 0.00123

131 <- 229 0.00170

131 <- 232 0.00158

132 <- 217 -0.00100

132 <- 239 -0.00165

132 <- 253 -0.00101

133 <- 212 0.00147

134 <- 258 0.00120

134 <- 261 -0.00148

135 <- 210 -0.00126

135 <- 213 -0.00144

135 <- 218 0.00109

136 <- 242 0.00125

137 <- 212 -0.00141

138 <- 210 0.00112

138 <- 243 -0.00104

138 <- 250 -0.00224

138 <- 271 0.00106

139 <- 237 -0.00127

139 <- 241 0.00132

139 <- 282 -0.00121

140 <- 223 -0.00119

140 <- 228 0.00103

140 <- 253 0.00125

140 <- 265 0.00122

141 <- 192 -0.00401

141 <- 199 -0.00154

141 <- 221 0.00136

141 <- 295 -0.00125

142 <- 223 -0.00119

143 <- 219 0.00112

143 <- 224 0.00176

144 <- 250 -0.00164

144 <- 259 0.00105

145 <- 228 -0.00113

145 <- 253 0.00240

145 <- 262 0.00117

145 <- 265 0.00235

146 <- 234 0.00110

146 <- 300 0.00110

148 <- 193 0.00123

148 <- 205 -0.00116

148 <- 207 0.00151

148 <- 298 -0.00116

148 <- 299 -0.00115

150 <- 191 0.00509

150 <- 200 0.00175

150 <- 233 -0.00186

151 <- 192 -0.00431

151 <- 199 -0.00121

151 <- 221 0.00163

152 <- 212 -0.00113

152 <- 236 -0.00118

152 <- 240 0.00147

152 <- 254 0.00114

153 <- 263 0.00100

153 <- 282 0.00194

154 <- 210 -0.00119

154 <- 215 -0.00104

154 <- 238 -0.00211

154 <- 243 -0.00200

155 <- 236 0.00127

155 <- 261 0.00170

156 <- 253 -0.00153

157 <- 250 0.00177

157 <- 259 -0.00141

158 <- 230 -0.00109

158 <- 237 -0.00104

158 <- 269 0.00109

159 <- 239 0.00126

159 <- 253 0.00166

159 <- 265 0.00164

160 <- 197 -0.00132

160 <- 315 -0.00128

161 <- 193 0.00153

161 <- 194 0.00160

161 <- 202 -0.00148

161 <- 314 -0.00113

162 <- 282 0.00113

162 <- 290 -0.00109

163 <- 201 0.00135

163 <- 205 0.00186

163 <- 210 0.00142

163 <- 215 0.00210

163 <- 225 -0.00205

163 <- 229 -0.00102

163 <- 232 0.00129

163 <- 243 0.00217

163 <- 266 -0.00107

164 <- 222 -0.00170

164 <- 227 -0.00177

165 <- 209 -0.00118

165 <- 216 0.00134

165 <- 222 0.00159

165 <- 261 0.00145

166 <- 192 -0.00515

166 <- 234 -0.00143

167 <- 198 0.00109

167 <- 242 -0.00269

167 <- 256 -0.00134

167 <- 263 -0.00110

167 <- 290 -0.00211

167 <- 361 0.00106

168 <- 201 0.00237

168 <- 205 0.00285

168 <- 215 0.00274

168 <- 218 -0.00189

168 <- 225 0.00148

168 <- 238 -0.00116

168 <- 243 0.00246

168 <- 252 -0.00174

168 <- 259 0.00105

168 <- 271 0.00189

168 <- 275 -0.00122

168 <- 285 -0.00101

169 <- 192 -0.00403

169 <- 196 0.00135

169 <- 199 -0.00379

169 <- 221 0.00237

169 <- 324 -0.00101

170 <- 194 -0.00372

170 <- 201 -0.00253

170 <- 207 0.00284

170 <- 215 0.00165

170 <- 255 -0.00152

171 <- 197 0.00119

171 <- 198 0.00359

171 <- 206 -0.00141

171 <- 226 0.00184

171 <- 231 -0.00120

171 <- 247 0.00129

171 <- 315 -0.00114

172 <- 244 -0.00214

172 <- 261 -0.00165

173 <- 191 0.00391

173 <- 195 0.00306

173 <- 204 0.00322

173 <- 220 -0.00113

173 <- 321 -0.00169

174 <- 191 0.00298

174 <- 195 0.00206

174 <- 204 0.00293

174 <- 220 -0.00169

174 <- 249 -0.00100

174 <- 321 0.00104

174 <- 325 -0.00103

175 <- 202 0.00124

175 <- 205 0.00264

175 <- 207 0.00272

175 <- 229 -0.00107

176 <- 198 -0.00256

176 <- 206 0.00167

176 <- 226 -0.00172

176 <- 246 0.00164

176 <- 335 0.00134

177 <- 201 -0.00129

177 <- 205 -0.00169

177 <- 215 -0.00231

177 <- 218 0.00119

177 <- 238 -0.00177

177 <- 250 -0.00146

177 <- 252 -0.00511

177 <- 259 0.00101

177 <- 275 0.00106

177 <- 285 -0.00101

177 <- 302 -0.00130

178 <- 242 0.00277

178 <- 251 -0.00148

178 <- 256 0.00131

178 <- 272 -0.00117

178 <- 290 0.00201

179 <- 209 0.00163

179 <- 216 0.00138

179 <- 244 0.00384

179 <- 254 0.00205

179 <- 258 0.00309

179 <- 264 -0.00134

179 <- 268 -0.00111

179 <- 274 0.00212

179 <- 283 0.00153

179 <- 312 0.00133

179 <- 324 -0.00111

179 <- 398 0.00101

180 <- 239 -0.00204

180 <- 245 -0.00204

180 <- 262 0.00170

180 <- 265 -0.00318

180 <- 273 0.00133

180 <- 277 0.00113

180 <- 296 -0.00135

181 <- 192 0.03478

181 <- 196 0.00230

181 <- 199 0.00905

181 <- 203 0.00404

181 <- 221 -0.00274

181 <- 234 -0.00329

181 <- 248 -0.00186

182 <- 192 -0.03529

182 <- 196 -0.00568

182 <- 199 -0.00475

182 <- 221 0.00121

183 <- 197 0.00475

183 <- 198 0.00496

183 <- 206 -0.00196

183 <- 226 0.00335

183 <- 231 -0.00315

183 <- 246 -0.00110

183 <- 247 0.00127

184 <- 201 -0.00316

184 <- 202 -0.00210

184 <- 205 -0.00124

184 <- 207 0.00167

184 <- 215 0.00106

184 <- 229 0.00146

184 <- 232 0.00135

184 <- 255 -0.00121

185 <- 191 -0.01624

185 <- 195 -0.00614

185 <- 220 0.00143

185 <- 350 0.00172

186 <- 192 0.00155

186 <- 199 0.00594

186 <- 221 -0.00342

186 <- 234 -0.00157

186 <- 248 -0.00119

187 <- 194 0.00327

187 <- 202 0.00219

187 <- 205 -0.00178

187 <- 207 -0.00607

187 <- 229 0.00129

187 <- 232 0.00117

188 <- 197 -0.00664

188 <- 198 0.00750

188 <- 226 0.00241

188 <- 354 0.00147

188 <- 364 -0.00146

189 <- 191 0.00607

189 <- 195 0.00327

189 <- 200 0.00560

189 <- 204 0.00281

189 <- 220 -0.00264

189 <- 350 0.00121

190 <- 191 -0.07645

190 <- 195 -0.00646

190 <- 200 -0.00739

190 <- 204 -0.00223

190 <- 233 0.00112

190 <- 375 0.00161

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

Total Energy, E(TD-HF/TD-KS) = -2348.10216210

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

Excited State 2: Singlet-B1 1.6973 eV 730.49 nm f=0.8637 <S\*\*2>=0.000

62 -> 282 0.00120

68 -> 262 -0.00101

77 -> 244 0.00105

86 -> 252 -0.00164

93 -> 253 0.00113

93 -> 262 0.00146

95 -> 252 0.00125

96 -> 258 0.00106

96 -> 264 -0.00102

98 -> 225 -0.00104

101 -> 264 -0.00196

101 -> 276 0.00126

101 -> 346 0.00123

106 -> 258 0.00103

107 -> 242 -0.00232

107 -> 251 0.00105

107 -> 256 -0.00159

107 -> 260 0.00107

107 -> 290 -0.00187

107 -> 361 0.00201

107 -> 393 -0.00163

108 -> 243 -0.00133

108 -> 252 -0.00246

108 -> 266 -0.00188

108 -> 275 -0.00143

109 -> 253 0.00120

110 -> 238 -0.00131

110 -> 243 -0.00131

110 -> 250 0.00144

111 -> 290 -0.00152

112 -> 254 0.00146

112 -> 274 0.00113

112 -> 385 0.00101

114 -> 210 -0.00116

114 -> 213 0.00139

114 -> 215 0.00101

114 -> 250 0.00129

115 -> 262 0.00138

116 -> 211 0.00154

117 -> 209 0.00148

117 -> 240 -0.00166

117 -> 244 0.00284

117 -> 258 0.00229

117 -> 264 -0.00196

117 -> 276 0.00114

117 -> 292 -0.00100

117 -> 346 -0.00116

117 -> 403 0.00103

118 -> 211 0.00138

118 -> 223 -0.00123

118 -> 235 -0.00115

119 -> 218 -0.00245

119 -> 243 0.00106

119 -> 250 0.00190

120 -> 242 0.00130

120 -> 282 0.00116

121 -> 209 -0.00127

121 -> 244 -0.00273

121 -> 254 -0.00135

121 -> 261 -0.00210

121 -> 346 0.00108

122 -> 195 -0.00223

122 -> 204 -0.00133

122 -> 220 -0.00281

122 -> 233 0.00282

122 -> 296 -0.00155

123 -> 216 -0.00219

123 -> 236 0.00110

123 -> 254 0.00109

124 -> 250 0.00114

125 -> 214 -0.00288

125 -> 219 0.00222

125 -> 230 0.00164

126 -> 209 0.00136

126 -> 216 -0.00264

126 -> 227 0.00121

127 -> 253 0.00149

128 -> 197 0.00142

128 -> 206 0.00135

128 -> 214 -0.00137

128 -> 251 -0.00103

129 -> 193 -0.00121

129 -> 194 -0.00108

129 -> 201 -0.00161

129 -> 205 -0.00130

129 -> 207 -0.00129

129 -> 250 0.00143

130 -> 193 0.00242

130 -> 194 0.00207

130 -> 201 0.00260

130 -> 202 -0.00195

130 -> 205 0.00163

130 -> 207 0.00253

130 -> 215 -0.00164

130 -> 229 -0.00183

130 -> 232 -0.00170

130 -> 317 -0.00105

130 -> 344 -0.00118

131 -> 197 0.00283

131 -> 206 0.00274

131 -> 231 0.00175

132 -> 216 0.00132

132 -> 240 0.00210

132 -> 254 0.00125

133 -> 211 -0.00195

133 -> 245 0.00115

134 -> 245 0.00107

134 -> 257 -0.00147

134 -> 262 -0.00178

135 -> 242 0.00155

136 -> 210 -0.00168

136 -> 213 0.00192

136 -> 218 0.00146

136 -> 243 -0.00112

136 -> 259 -0.00113

137 -> 211 -0.00189

137 -> 245 -0.00122

138 -> 214 0.00117

138 -> 224 -0.00105

138 -> 237 -0.00161

138 -> 241 -0.00167

138 -> 282 -0.00140

139 -> 210 0.00148

139 -> 243 -0.00126

139 -> 250 -0.00276

139 -> 259 -0.00115

139 -> 271 0.00126

139 -> 279 0.00108

140 -> 222 -0.00156

140 -> 227 0.00135

140 -> 254 0.00154

140 -> 264 0.00149

141 -> 191 -0.00738

141 -> 200 -0.00214

141 -> 220 0.00121

141 -> 296 0.00153

142 -> 222 0.00157

142 -> 227 -0.00108

142 -> 240 0.00124

142 -> 254 -0.00118

143 -> 210 0.00116

143 -> 250 -0.00204

143 -> 259 -0.00130

144 -> 219 -0.00149

144 -> 224 0.00231

144 -> 230 0.00130

144 -> 241 0.00115

144 -> 303 -0.00112

145 -> 227 -0.00146

145 -> 240 0.00110

145 -> 254 0.00295

145 -> 261 0.00138

145 -> 264 0.00288

146 -> 233 -0.00129

146 -> 301 0.00131

147 -> 193 0.00187

147 -> 205 0.00175

147 -> 207 0.00196

147 -> 229 -0.00104

147 -> 298 -0.00143

147 -> 299 0.00139

148 -> 206 0.00117

148 -> 231 0.00118

150 -> 192 -0.00703

150 -> 196 0.00102

150 -> 199 -0.00279

150 -> 234 0.00183

150 -> 295 0.00125

151 -> 191 -0.00806

151 -> 200 -0.00157

151 -> 204 -0.00121

151 -> 220 0.00149

151 -> 301 0.00126

152 -> 211 0.00156

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Excited State 3: Singlet-A2 2.5943 eV 477.90 nm f=0.0000 <S\*\*2>=0.000

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168 <- 245 0.00131

168 <- 257 0.00105

169 <- 198 -0.00369

170 <- 191 0.00511

170 <- 195 0.00228

170 <- 200 0.00223

170 <- 204 0.00327

170 <- 220 -0.00105

171 <- 192 0.00506

171 <- 196 0.00228

171 <- 199 0.00225

171 <- 203 0.00325

171 <- 221 -0.00105

173 <- 193 -0.00287

173 <- 202 0.00341

173 <- 207 0.00429

173 <- 298 0.00121

174 <- 194 -0.00332

174 <- 201 -0.00383

174 <- 205 0.00335

174 <- 299 -0.00101

175 <- 191 -0.00506

175 <- 195 0.00157

175 <- 200 -0.00215

175 <- 204 0.00380

176 <- 192 -0.00509

176 <- 196 0.00160

176 <- 199 -0.00214

176 <- 203 0.00378

177 <- 191 -0.00102

177 <- 265 0.00126

178 <- 264 -0.00126

179 <- 251 0.00100

179 <- 260 0.00121

180 <- 250 0.00152

181 <- 197 -0.00127

181 <- 206 -0.00463

181 <- 231 -0.00323

182 <- 197 0.00814

182 <- 231 -0.00177

183 <- 196 -0.00105

183 <- 199 0.00612

183 <- 203 0.00209

183 <- 221 -0.00187

183 <- 234 -0.00292

184 <- 195 -0.00103

184 <- 200 0.00610

184 <- 204 0.00209

184 <- 220 -0.00186

184 <- 233 -0.00293

185 <- 193 0.00304

185 <- 202 0.00236

185 <- 207 -0.00352

186 <- 198 0.00782

186 <- 226 0.00404

187 <- 191 0.00549

187 <- 195 -0.00723

187 <- 204 -0.00123

187 <- 220 0.00140

187 <- 233 -0.00127

188 <- 192 0.00549

188 <- 196 -0.00722

188 <- 203 -0.00123

188 <- 221 0.00141

188 <- 234 -0.00128

189 <- 194 -0.00885

189 <- 205 0.00165

190 <- 193 -0.01383

190 <- 202 0.00442

190 <- 207 -0.00236

190 <- 347 0.00111

190 <- 381 -0.00123

Excited State 4: Singlet-A2 2.6738 eV 463.70 nm f=0.0000 <S\*\*2>=0.000

84 -> 238 -0.00101

93 -> 282 0.00113

97 -> 219 0.00121

98 -> 216 -0.00117

99 -> 217 0.00117

100 -> 214 0.00128

109 -> 241 -0.00107

112 -> 238 0.00128

117 -> 218 -0.00103

117 -> 266 -0.00104

118 -> 214 -0.00122

119 -> 240 -0.00113

120 -> 239 -0.00112

121 -> 250 -0.00101

121 -> 278 -0.00105

123 -> 213 0.00115

123 -> 225 -0.00139

124 -> 212 0.00109

124 -> 222 0.00115

125 -> 211 -0.00109

125 -> 223 -0.00115

126 -> 210 -0.00169

126 -> 218 -0.00145

127 -> 251 -0.00127

127 -> 260 0.00100

128 -> 191 -0.00143

129 -> 192 -0.00142

130 -> 192 0.00277

131 -> 191 -0.00279

132 -> 297 -0.00133

132 -> 316 -0.00119

133 -> 251 0.00113

134 -> 256 -0.00120

141 -> 197 0.00151

142 -> 285 -0.00109

143 -> 283 0.00124

144 -> 284 0.00124

147 -> 192 0.00423

147 -> 196 0.00154

148 -> 191 -0.00425

148 -> 195 -0.00155

150 -> 193 0.00301

150 -> 207 -0.00467

151 -> 197 0.00380

152 -> 251 0.00133

155 -> 357 -0.00124

156 -> 259 -0.00191

156 -> 279 -0.00128

156 -> 285 0.00151

157 -> 253 -0.00137

157 -> 273 -0.00174

157 -> 284 -0.00129

158 -> 254 -0.00137

158 -> 274 0.00174

158 -> 283 -0.00129

159 -> 250 -0.00109

159 -> 266 -0.00150

159 -> 271 -0.00116

159 -> 278 -0.00184

159 -> 334 -0.00122

160 -> 196 -0.00484

160 -> 199 -0.00362

160 -> 203 -0.00445

160 -> 221 0.00174

161 -> 195 -0.00483

161 -> 200 -0.00364

161 -> 204 -0.00445

161 -> 220 0.00172

164 -> 260 0.00134

164 -> 369 -0.00101

165 -> 282 -0.00103

166 -> 198 0.00486

167 -> 196 -0.00187

167 -> 244 0.00142

167 -> 258 0.00115

168 -> 195 -0.00187

168 -> 245 -0.00142

168 -> 257 -0.00114

169 -> 197 -0.00158

169 -> 206 0.00225

170 -> 191 -0.00502

170 -> 195 0.00714

170 -> 200 -0.00247

170 -> 204 0.00413

170 -> 220 -0.00143

171 -> 192 0.00503

171 -> 196 -0.00714

171 -> 199 0.00245

171 -> 203 -0.00415

171 -> 221 0.00143

173 -> 194 -0.00834

173 -> 201 -0.00726

173 -> 205 0.00539

173 -> 299 -0.00160

174 -> 193 -0.00449

174 -> 202 0.00779

174 -> 207 0.00223

174 -> 298 0.00154

175 -> 191 -0.00305

175 -> 195 -0.00290

175 -> 200 -0.00366

175 -> 204 0.00482

176 -> 192 0.00304

176 -> 196 0.00288

176 -> 199 0.00366

176 -> 203 -0.00484

177 -> 195 -0.00101

178 -> 196 -0.00101

179 -> 197 0.00107

179 -> 242 -0.00194

179 -> 256 -0.00154

181 -> 198 0.00482

181 -> 226 0.00178

182 -> 198 0.01036

182 -> 226 0.00433

183 -> 192 -0.02319

183 -> 196 -0.00660

183 -> 199 0.00963

183 -> 203 0.00255

183 -> 221 -0.00249

183 -> 234 -0.00321

184 -> 191 0.02325

184 -> 195 0.00666

184 -> 200 -0.00963

184 -> 204 -0.00254

184 -> 220 0.00251

184 -> 233 0.00322

185 -> 194 0.03040

185 -> 201 0.00614

185 -> 205 -0.00267

185 -> 317 0.00109

186 -> 197 0.01812

186 -> 206 -0.00375

186 -> 231 -0.00412

187 -> 191 0.03932

187 -> 200 0.00422

187 -> 204 -0.00481

188 -> 192 -0.03941

188 -> 199 -0.00420

188 -> 203 0.00483

189 -> 193 -0.01426

189 -> 202 0.00731

189 -> 298 0.00119

189 -> 314 0.00109

189 -> 381 -0.00104

190 -> 194 0.70223

190 -> 201 0.01704

190 -> 229 -0.00206

190 -> 232 -0.00171

190 -> 344 0.00124

126 <- 210 -0.00109

130 <- 192 0.00150

131 <- 191 -0.00152

132 <- 297 -0.00103

147 <- 192 0.00270

148 <- 191 -0.00272

150 <- 207 -0.00274

151 <- 197 0.00254

156 <- 259 -0.00136

156 <- 285 0.00107

157 <- 273 -0.00127

158 <- 274 0.00127

159 <- 266 -0.00106

159 <- 278 -0.00130

160 <- 192 -0.00185

160 <- 199 -0.00273

160 <- 203 -0.00177

160 <- 221 0.00122

161 <- 191 -0.00187

161 <- 200 -0.00274

161 <- 204 -0.00177

161 <- 220 0.00121

166 <- 198 0.00352

169 <- 206 0.00256

170 <- 191 -0.00140

170 <- 195 0.00105

170 <- 200 -0.00142

170 <- 204 0.00118

170 <- 220 -0.00163

171 <- 192 0.00142

171 <- 196 -0.00105

171 <- 199 0.00142

171 <- 203 -0.00119

171 <- 221 0.00164

173 <- 194 -0.00330

173 <- 201 -0.00318

173 <- 205 0.00309

173 <- 229 -0.00111

173 <- 299 -0.00115

174 <- 193 -0.00327

174 <- 202 0.00420

174 <- 207 0.00227

174 <- 298 0.00109

175 <- 191 -0.00108

175 <- 195 0.00262

175 <- 200 -0.00166

175 <- 204 0.00402

176 <- 192 0.00115

176 <- 196 -0.00260

176 <- 199 0.00165

176 <- 203 -0.00404

179 <- 242 -0.00119

179 <- 256 -0.00102

181 <- 198 0.00302

181 <- 226 0.00151

182 <- 198 0.00582

182 <- 226 0.00288

183 <- 196 -0.00153

183 <- 199 0.00505

183 <- 203 0.00188

183 <- 221 -0.00119

183 <- 234 -0.00250

184 <- 195 0.00150

184 <- 200 -0.00504

184 <- 204 -0.00187

184 <- 220 0.00120

184 <- 233 0.00250

185 <- 194 0.00416

185 <- 201 -0.00119

186 <- 197 0.00441

186 <- 206 -0.00328

186 <- 231 -0.00294

187 <- 191 0.00291

187 <- 195 -0.00777

187 <- 204 -0.00144

188 <- 192 -0.00291

188 <- 196 0.00778

188 <- 203 0.00145

189 <- 193 -0.00851

189 <- 207 0.00175

190 <- 194 -0.01140

190 <- 201 -0.00223

190 <- 205 0.00212

190 <- 377 0.00106

Excited State 5: Singlet-B2 2.7836 eV 445.40 nm f=0.0413 <S\*\*2>=0.000

93 -> 261 0.00100

97 -> 216 -0.00103

98 -> 214 -0.00133

98 -> 219 0.00105

100 -> 216 0.00101

108 -> 242 -0.00152

111 -> 218 0.00104

119 -> 241 0.00115

120 -> 238 -0.00105

121 -> 265 -0.00122

122 -> 192 -0.00256

123 -> 223 -0.00109

125 -> 210 -0.00149

125 -> 218 -0.00107

125 -> 225 -0.00129

126 -> 208 -0.00120

126 -> 217 -0.00133

126 -> 223 -0.00104

127 -> 258 -0.00116

131 -> 194 -0.00130

131 -> 207 0.00149

132 -> 265 0.00102

138 -> 297 -0.00106

141 -> 196 0.00108

142 -> 284 -0.00116

144 -> 278 0.00102

144 -> 285 0.00105

146 -> 192 0.00391

147 -> 197 0.00187

148 -> 207 0.00192

150 -> 191 0.00525

150 -> 195 0.00473

150 -> 200 0.00213

150 -> 204 0.00299

150 -> 220 -0.00216

151 -> 192 0.00290

151 -> 196 0.00148

151 -> 199 -0.00193

151 -> 203 -0.00109

152 -> 240 0.00119

152 -> 244 -0.00115

153 -> 224 -0.00103

153 -> 251 0.00107

153 -> 327 0.00104

153 -> 357 -0.00115

156 -> 253 0.00104

156 -> 273 0.00174

156 -> 284 0.00121

157 -> 259 0.00150

157 -> 266 -0.00142

157 -> 271 -0.00106

157 -> 278 -0.00151

157 -> 279 0.00128

157 -> 285 -0.00133

157 -> 334 -0.00107

159 -> 253 -0.00103

159 -> 273 -0.00158

159 -> 284 -0.00122

160 -> 197 0.00279

160 -> 198 0.00472

160 -> 206 -0.00151

160 -> 226 0.00105

161 -> 193 -0.00475

161 -> 194 -0.00544

161 -> 201 -0.00196

161 -> 205 0.00241

161 -> 207 0.00490

163 -> 205 0.00109

166 -> 192 -0.00361

166 -> 199 -0.00443

166 -> 203 -0.00143

166 -> 221 0.00110

167 -> 256 0.00108

167 -> 260 -0.00137

168 -> 193 -0.00131

168 -> 194 -0.00167

168 -> 205 0.00199

168 -> 215 0.00100

169 -> 192 0.00102

169 -> 199 0.00189

170 -> 193 0.00700

170 -> 194 0.00719

170 -> 201 0.00268

170 -> 202 -0.00360

170 -> 205 -0.00381

170 -> 207 -0.00281

170 -> 215 0.00126

170 -> 229 0.00113

171 -> 206 0.00108

172 -> 264 0.00118

173 -> 191 0.00700

173 -> 195 -0.00601

173 -> 200 0.00258

173 -> 204 -0.00815

173 -> 220 0.00158

173 -> 296 0.00119

174 -> 191 0.00929

174 -> 195 -0.00206

174 -> 200 0.00436

174 -> 204 -0.00660

175 -> 193 -0.00117

175 -> 194 -0.00353

175 -> 201 0.00508

175 -> 202 -0.00692

175 -> 205 -0.00235

175 -> 298 -0.00113

175 -> 299 0.00113

176 -> 197 0.00139

176 -> 198 -0.00224

176 -> 226 -0.00138

176 -> 247 0.00101

177 -> 194 -0.00133

177 -> 252 -0.00167

179 -> 192 0.00226

180 -> 191 -0.00221

181 -> 192 0.04493

181 -> 196 0.00276

181 -> 234 0.00157

182 -> 192 -0.01323

182 -> 196 0.00420

182 -> 199 -0.01121

182 -> 203 -0.00220

182 -> 221 0.00437

182 -> 222 0.00106

182 -> 234 0.00154

183 -> 197 -0.01638

183 -> 198 -0.01049

183 -> 206 0.00281

183 -> 226 -0.00368

183 -> 231 0.00319

184 -> 193 0.00143

184 -> 201 -0.00161

184 -> 202 -0.00171

185 -> 191 -0.02380

185 -> 195 0.02641

185 -> 204 0.00720

186 -> 192 0.03137

186 -> 196 0.00567

186 -> 199 -0.00766

186 -> 203 -0.00335

186 -> 221 0.00118

186 -> 234 0.00317

187 -> 193 -0.01036

187 -> 194 -0.00136

187 -> 201 -0.00526

187 -> 202 0.00891

187 -> 205 0.00302

187 -> 207 -0.00252

187 -> 317 -0.00121

188 -> 197 -0.00964

188 -> 198 0.00768

188 -> 206 0.00125

188 -> 226 0.00130

188 -> 231 0.00124

189 -> 191 0.10132

189 -> 195 -0.01006

189 -> 200 0.01021

189 -> 204 -0.00412

189 -> 220 -0.00111

190 -> 191 0.01640

190 -> 195 0.69508

190 -> 200 -0.00661

190 -> 204 0.01150

190 -> 220 0.00281

108 <- 242 -0.00112

122 <- 192 -0.00139

146 <- 192 0.00235

147 <- 197 0.00135

148 <- 207 0.00115

150 <- 191 0.00382

150 <- 200 0.00123

150 <- 220 -0.00114

151 <- 192 0.00191

151 <- 196 0.00104

151 <- 199 -0.00110

156 <- 273 0.00126

157 <- 259 0.00105

157 <- 266 -0.00100

157 <- 278 -0.00105

159 <- 273 -0.00114

160 <- 197 0.00190

160 <- 198 0.00284

160 <- 206 -0.00101

161 <- 207 0.00265

166 <- 192 -0.00284

166 <- 199 -0.00303

166 <- 203 -0.00109

169 <- 192 0.00197

169 <- 199 0.00159

169 <- 203 0.00100

169 <- 221 0.00113

170 <- 202 -0.00114

170 <- 205 -0.00138

170 <- 207 -0.00162

171 <- 197 0.00123

171 <- 198 -0.00118

171 <- 206 0.00195

173 <- 195 -0.00243

173 <- 204 -0.00378

173 <- 220 0.00148

174 <- 191 0.00223

174 <- 195 -0.00229

174 <- 200 0.00153

174 <- 204 -0.00394

175 <- 193 0.00281

175 <- 194 0.00246

175 <- 201 0.00308

175 <- 202 -0.00379

175 <- 205 -0.00222

176 <- 197 -0.00130

181 <- 192 0.00380

181 <- 199 -0.00107

181 <- 234 0.00136

182 <- 192 -0.00489

182 <- 196 0.00101

182 <- 199 -0.00553

182 <- 203 -0.00136

182 <- 221 0.00227

182 <- 234 0.00120

183 <- 197 -0.00327

183 <- 198 -0.00582

183 <- 206 0.00296

183 <- 226 -0.00258

183 <- 231 0.00236

185 <- 191 -0.00156

185 <- 195 0.00315

185 <- 200 0.00141

185 <- 220 -0.00118

186 <- 199 -0.00418

186 <- 203 -0.00210

186 <- 234 0.00241

187 <- 193 -0.00785

187 <- 194 -0.00749

187 <- 205 0.00109

188 <- 198 0.00154

189 <- 191 0.00541

189 <- 195 -0.00711

190 <- 191 -0.00522

190 <- 195 -0.01113

190 <- 204 -0.00326

Excited State 6: Singlet-B1 2.7836 eV 445.40 nm f=0.0413 <S\*\*2>=0.000

93 -> 262 0.00100

97 -> 217 0.00103

99 -> 214 0.00133

99 -> 219 0.00105

100 -> 217 0.00101

107 -> 242 -0.00152

110 -> 218 0.00104

119 -> 238 0.00105

120 -> 241 -0.00115

121 -> 264 -0.00122

122 -> 191 0.00256

123 -> 222 0.00109

124 -> 210 0.00149

124 -> 218 0.00107

124 -> 225 -0.00129

126 -> 209 0.00120

126 -> 216 -0.00133

126 -> 222 -0.00104

127 -> 257 -0.00116

130 -> 194 0.00130

130 -> 207 0.00149

132 -> 264 -0.00102

139 -> 297 0.00106

141 -> 195 0.00108

142 -> 283 0.00116

143 -> 278 0.00102

143 -> 285 -0.00105

146 -> 191 -0.00391

147 -> 207 0.00192

148 -> 197 -0.00187

150 -> 192 -0.00525

150 -> 196 -0.00473

150 -> 199 -0.00213

150 -> 203 -0.00299

150 -> 221 0.00216

151 -> 191 0.00290

151 -> 195 0.00148

151 -> 200 -0.00193

151 -> 204 -0.00109

152 -> 239 -0.00119

152 -> 245 -0.00115

154 -> 224 0.00103

154 -> 251 0.00107

154 -> 327 0.00104

154 -> 357 0.00115

156 -> 254 -0.00104

156 -> 274 0.00174

156 -> 283 -0.00121

158 -> 259 -0.00150

158 -> 266 -0.00142

158 -> 271 -0.00106

158 -> 278 -0.00151

158 -> 279 -0.00128

158 -> 285 0.00133

158 -> 334 -0.00107

159 -> 254 -0.00103

159 -> 274 0.00158

159 -> 283 -0.00122

160 -> 193 0.00475

160 -> 194 -0.00544

160 -> 201 -0.00196

160 -> 205 0.00241

160 -> 207 -0.00490

161 -> 197 0.00279

161 -> 198 -0.00472

161 -> 206 -0.00151

161 -> 226 -0.00105

162 -> 205 0.00109

166 -> 191 0.00361

166 -> 200 0.00443

166 -> 204 0.00143

166 -> 220 -0.00110

167 -> 193 0.00131

167 -> 194 -0.00167

167 -> 205 0.00199

167 -> 215 0.00100

168 -> 256 0.00108

168 -> 260 0.00137

169 -> 191 0.00102

169 -> 200 0.00189

170 -> 206 -0.00108

171 -> 193 0.00700

171 -> 194 -0.00719

171 -> 201 -0.00268

171 -> 202 -0.00360

171 -> 205 0.00381

171 -> 207 -0.00281

171 -> 215 -0.00126

171 -> 229 -0.00113

172 -> 265 -0.00118

173 -> 192 0.00700

173 -> 196 -0.00601

173 -> 199 0.00258

173 -> 203 -0.00815

173 -> 221 0.00158

173 -> 295 -0.00119

174 -> 192 -0.00929

174 -> 196 0.00206

174 -> 199 -0.00436

174 -> 203 0.00660

175 -> 197 -0.00139

175 -> 198 -0.00224

175 -> 226 -0.00138

175 -> 247 -0.00101

176 -> 193 -0.00117

176 -> 194 0.00353

176 -> 201 -0.00508

176 -> 202 -0.00692

176 -> 205 0.00235

176 -> 298 -0.00113

176 -> 299 -0.00113

178 -> 194 -0.00133

178 -> 252 0.00167

179 -> 191 0.00226

180 -> 192 0.00221

181 -> 191 -0.04493

181 -> 195 -0.00276

181 -> 233 -0.00157

182 -> 191 0.01323

182 -> 195 -0.00420

182 -> 200 0.01121

182 -> 204 0.00220

182 -> 220 -0.00437

182 -> 223 -0.00106

182 -> 233 -0.00154

183 -> 193 0.00143

183 -> 201 0.00161

183 -> 202 -0.00171

184 -> 197 0.01638

184 -> 198 -0.01049

184 -> 206 -0.00281

184 -> 226 -0.00368

184 -> 231 -0.00319

185 -> 192 -0.02380

185 -> 196 0.02641

185 -> 203 0.00720

186 -> 191 0.03137

186 -> 195 0.00567

186 -> 200 -0.00766

186 -> 204 -0.00335

186 -> 220 0.00118

186 -> 233 0.00317

187 -> 197 0.00964

187 -> 198 0.00768

187 -> 206 -0.00125

187 -> 226 0.00130

187 -> 231 -0.00124

188 -> 193 -0.01036

188 -> 194 0.00136

188 -> 201 0.00526

188 -> 202 0.00891

188 -> 205 -0.00302

188 -> 207 -0.00252

188 -> 317 0.00121

189 -> 192 -0.10132

189 -> 196 0.01006

189 -> 199 -0.01021

189 -> 203 0.00412

189 -> 221 0.00111

190 -> 192 0.01640

190 -> 196 0.69508

190 -> 199 -0.00661

190 -> 203 0.01150

190 -> 221 0.00281

107 <- 242 -0.00112

122 <- 191 0.00139

146 <- 191 -0.00235

147 <- 207 0.00115

148 <- 197 -0.00135

150 <- 192 -0.00382

150 <- 199 -0.00123

150 <- 221 0.00114

151 <- 191 0.00191

151 <- 195 0.00104

151 <- 200 -0.00110

156 <- 274 0.00126

158 <- 259 -0.00105

158 <- 266 -0.00100

158 <- 278 -0.00105

159 <- 274 0.00114

160 <- 207 -0.00265

161 <- 197 0.00190

161 <- 198 -0.00284

161 <- 206 -0.00101

166 <- 191 0.00284

166 <- 200 0.00303

166 <- 204 0.00109

169 <- 191 0.00197

169 <- 200 0.00159

169 <- 204 0.00100

169 <- 220 0.00113

170 <- 197 -0.00123

170 <- 198 -0.00118

170 <- 206 -0.00195

171 <- 202 -0.00114

171 <- 205 0.00138

171 <- 207 -0.00162

173 <- 196 -0.00243

173 <- 203 -0.00378

173 <- 221 0.00148

174 <- 192 -0.00223

174 <- 196 0.00229

174 <- 199 -0.00153

174 <- 203 0.00394

175 <- 197 0.00130

176 <- 193 0.00281

176 <- 194 -0.00246

176 <- 201 -0.00308

176 <- 202 -0.00379

176 <- 205 0.00221

181 <- 191 -0.00380

181 <- 200 0.00107

181 <- 233 -0.00136

182 <- 191 0.00489

182 <- 195 -0.00101

182 <- 200 0.00553

182 <- 204 0.00136

182 <- 220 -0.00227

182 <- 233 -0.00120

184 <- 197 0.00327

184 <- 198 -0.00582

184 <- 206 -0.00296

184 <- 226 -0.00258

184 <- 231 -0.00236

185 <- 192 -0.00156

185 <- 196 0.00315

185 <- 199 0.00141

185 <- 221 -0.00118

186 <- 200 -0.00418

186 <- 204 -0.00210

186 <- 233 0.00241

187 <- 198 0.00154

188 <- 193 -0.00785

188 <- 194 0.00749

188 <- 205 -0.00109

189 <- 192 -0.00541

189 <- 196 0.00711

190 <- 192 -0.00522

190 <- 196 -0.01113

190 <- 203 -0.00326

Excited State 7: Singlet-A2 2.9246 eV 423.93 nm f=0.0000 <S\*\*2>=0.000

126 -> 210 0.00113

130 -> 192 -0.00119

131 -> 191 0.00120

132 -> 297 0.00111

141 -> 197 -0.00110

146 -> 198 -0.00115

147 -> 192 -0.00219

147 -> 196 -0.00112

147 -> 199 0.00107

148 -> 191 0.00219

148 -> 195 0.00112

148 -> 200 -0.00107

150 -> 193 -0.00248

150 -> 202 0.00155

151 -> 197 -0.00441

156 -> 279 0.00104

157 -> 273 0.00121

158 -> 274 -0.00120

159 -> 278 0.00117

160 -> 192 -0.00546

160 -> 203 0.00145

161 -> 191 -0.00544

161 -> 204 0.00146

166 -> 198 -0.00193

167 -> 192 -0.00160

168 -> 191 -0.00160

169 -> 197 -0.00567

169 -> 206 -0.00405

170 -> 191 0.00922

170 -> 200 0.00176

170 -> 204 -0.00125

170 -> 220 0.00168

171 -> 192 -0.00920

171 -> 199 -0.00175

171 -> 203 0.00125

171 -> 221 -0.00168

173 -> 194 0.00540

173 -> 201 0.00386

173 -> 205 -0.00324

173 -> 229 0.00108

173 -> 299 0.00103

174 -> 193 0.00144

174 -> 202 -0.00220

174 -> 207 -0.00666

174 -> 298 -0.00111

175 -> 191 -0.02945

175 -> 195 -0.00610

175 -> 200 -0.00192

175 -> 204 -0.00554

175 -> 220 0.00183

176 -> 192 0.02943

176 -> 196 0.00610

176 -> 199 0.00191

176 -> 203 0.00553

176 -> 221 -0.00183

177 -> 191 -0.00914

178 -> 192 -0.00911

179 -> 197 -0.00219

181 -> 198 -0.00600

181 -> 226 -0.00193

182 -> 198 -0.00440

182 -> 226 -0.00230

183 -> 192 -0.00816

183 -> 196 0.00199

183 -> 199 -0.00749

183 -> 203 -0.00263

183 -> 221 0.00142

183 -> 234 0.00276

184 -> 191 0.00819

184 -> 195 -0.00198

184 -> 200 0.00748

184 -> 204 0.00263

184 -> 220 -0.00142

184 -> 233 -0.00277

185 -> 201 0.00100

185 -> 205 -0.00143

186 -> 197 -0.00482

186 -> 206 0.00534

186 -> 231 0.00358

187 -> 191 0.49657

187 -> 195 0.00642

187 -> 200 0.01085

187 -> 204 0.00233

187 -> 220 -0.00350

188 -> 192 -0.49619

188 -> 196 -0.00642

188 -> 199 -0.01086

188 -> 203 -0.00234

188 -> 221 0.00350

189 -> 193 -0.02646

189 -> 202 0.00879

189 -> 207 -0.01200

190 -> 194 -0.05663

190 -> 201 0.00189

190 -> 205 -0.00319

147 <- 192 -0.00122

148 <- 191 0.00123

151 <- 197 -0.00213

169 <- 206 -0.00118

170 <- 191 0.00214

170 <- 220 0.00103

171 <- 192 -0.00215

171 <- 221 -0.00103

173 <- 194 0.00193

173 <- 201 0.00217

173 <- 205 -0.00214

174 <- 193 0.00170

174 <- 202 -0.00281

174 <- 207 -0.00152

175 <- 195 -0.00114

175 <- 204 -0.00270

176 <- 196 0.00113

176 <- 203 0.00271

181 <- 198 -0.00277

181 <- 226 -0.00148

182 <- 198 -0.00160

182 <- 226 -0.00115

183 <- 192 0.00312

183 <- 196 0.00143

183 <- 199 -0.00261

183 <- 234 0.00139

184 <- 191 -0.00312

184 <- 195 -0.00142

184 <- 200 0.00261

184 <- 233 -0.00139

185 <- 194 -0.00350

185 <- 201 0.00110

186 <- 197 -0.00394

186 <- 206 0.00101

186 <- 231 0.00159

187 <- 191 -0.00346

187 <- 195 0.00501

188 <- 192 0.00346

188 <- 196 -0.00500

189 <- 193 0.00612

190 <- 194 0.00607

190 <- 201 0.00121

Excited State 8: Singlet-B2 2.9424 eV 421.37 nm f=0.3284 <S\*\*2>=0.000

107 -> 252 0.00101

112 -> 239 -0.00101

113 -> 210 0.00100

113 -> 213 0.00108

116 -> 212 0.00141

118 -> 212 -0.00121

118 -> 216 0.00104

119 -> 241 -0.00124

120 -> 213 -0.00110

120 -> 238 0.00117

122 -> 192 -0.00170

123 -> 217 -0.00133

123 -> 228 0.00127

124 -> 214 -0.00206

124 -> 219 -0.00151

124 -> 230 -0.00108

124 -> 251 0.00108

125 -> 210 0.00128

126 -> 208 0.00150

126 -> 217 0.00208

131 -> 193 0.00192

132 -> 239 0.00131

132 -> 257 -0.00124

133 -> 212 -0.00122

134 -> 212 -0.00111

137 -> 212 0.00107

138 -> 210 -0.00108

138 -> 297 0.00109

139 -> 237 0.00112

139 -> 241 -0.00119

139 -> 251 0.00101

140 -> 223 0.00128

140 -> 239 0.00142

141 -> 192 -0.00237

141 -> 196 0.00184

141 -> 203 0.00102

142 -> 223 0.00119

142 -> 239 0.00116

143 -> 219 -0.00155

143 -> 224 -0.00174

143 -> 251 -0.00115

147 -> 197 -0.00117

147 -> 198 -0.00111

148 -> 194 0.00108

148 -> 207 0.00102

148 -> 299 0.00101

150 -> 191 -0.00232

150 -> 195 -0.00249

150 -> 204 -0.00114

151 -> 192 -0.00444

152 -> 236 0.00113

152 -> 254 0.00153

154 -> 225 0.00106

154 -> 232 -0.00125

154 -> 250 0.00140

154 -> 286 -0.00125

154 -> 287 -0.00100

154 -> 297 0.00110

155 -> 227 0.00161

155 -> 236 -0.00101

156 -> 235 -0.00120

156 -> 257 -0.00107

156 -> 273 -0.00102

158 -> 230 0.00127

158 -> 237 0.00137

158 -> 256 0.00107

158 -> 260 0.00135

159 -> 273 0.00113

160 -> 197 -0.00452

161 -> 193 -0.00229

161 -> 194 0.00543

161 -> 201 0.00174

161 -> 205 -0.00208

163 -> 210 -0.00109

163 -> 218 -0.00121

163 -> 225 0.00190

164 -> 222 0.00179

164 -> 227 0.00124

165 -> 209 0.00117

165 -> 216 -0.00116

165 -> 222 -0.00131

166 -> 196 -0.00376

166 -> 199 0.00137

166 -> 203 -0.00158

166 -> 221 0.00135

168 -> 205 -0.00108

168 -> 218 0.00131

169 -> 192 -0.00165

169 -> 196 -0.00283

169 -> 203 -0.00258

170 -> 194 -0.00111

170 -> 207 0.00513

171 -> 197 -0.00556

171 -> 206 -0.00364

172 -> 264 -0.00186

173 -> 195 0.00365

173 -> 200 -0.00185

173 -> 204 0.00340

173 -> 220 -0.00252

173 -> 233 0.00155

174 -> 191 0.01919

174 -> 195 0.00358

174 -> 200 0.00407

174 -> 204 0.00575

174 -> 220 -0.00176

174 -> 321 -0.00142

175 -> 193 -0.00324

175 -> 194 -0.00183

175 -> 201 -0.00318

175 -> 202 0.00251

175 -> 205 0.00225

175 -> 207 0.00266

175 -> 229 -0.00139

175 -> 232 -0.00118

176 -> 197 0.00533

176 -> 198 -0.00361

176 -> 206 -0.00136

176 -> 315 0.00117

176 -> 322 0.00102

177 -> 218 0.00100

177 -> 238 0.00114

177 -> 252 0.00113

178 -> 214 -0.00126

179 -> 192 -0.00283

179 -> 254 -0.00112

180 -> 191 -0.00975

180 -> 200 -0.00116

180 -> 217 0.00121

180 -> 239 0.00106

181 -> 192 0.01920

181 -> 196 -0.00953

181 -> 199 0.00264

181 -> 221 0.00146

181 -> 234 -0.00313

182 -> 192 -0.00970

182 -> 196 -0.02566

182 -> 199 0.00261

182 -> 203 -0.00156

182 -> 221 -0.00179

183 -> 197 0.00756

183 -> 198 0.00620

183 -> 206 -0.00178

183 -> 226 0.00258

183 -> 231 -0.00248

184 -> 193 -0.02640

184 -> 194 0.02764

184 -> 201 0.00118

184 -> 205 -0.00174

184 -> 207 0.00348

185 -> 191 0.00756

185 -> 195 0.00458

185 -> 200 -0.00897

185 -> 204 -0.00138

185 -> 220 0.00225

185 -> 233 -0.00131

185 -> 249 -0.00111

186 -> 192 -0.05410

186 -> 196 0.02158

186 -> 199 0.00529

186 -> 203 0.00388

186 -> 221 -0.00257

186 -> 234 -0.00119

187 -> 193 -0.01898

187 -> 194 -0.00264

187 -> 202 0.00493

187 -> 207 -0.00742

187 -> 229 0.00131

187 -> 232 0.00117

187 -> 255 0.00123

188 -> 197 0.02853

188 -> 198 -0.00787

188 -> 231 0.00113

188 -> 247 -0.00148

188 -> 354 -0.00130

189 -> 191 0.69391

189 -> 195 0.01073

189 -> 200 0.00356

189 -> 220 -0.00302

189 -> 249 -0.00126

189 -> 350 -0.00107

190 -> 191 -0.01397

190 -> 195 -0.09951

190 -> 200 -0.00635

190 -> 220 0.00139

190 -> 233 0.00105

124 <- 214 -0.00128

126 <- 217 0.00130

131 <- 193 0.00110

141 <- 192 -0.00142

141 <- 196 0.00121

143 <- 224 -0.00109

150 <- 191 -0.00260

150 <- 195 -0.00126

151 <- 192 -0.00245

152 <- 254 0.00104

160 <- 197 -0.00208

161 <- 193 -0.00189

161 <- 194 0.00273

161 <- 201 0.00116

161 <- 205 -0.00123

163 <- 225 0.00108

164 <- 222 0.00102

166 <- 196 -0.00214

166 <- 199 0.00103

166 <- 203 -0.00101

169 <- 192 -0.00170

169 <- 196 -0.00150

169 <- 203 -0.00151

170 <- 207 0.00212

171 <- 206 -0.00116

172 <- 264 -0.00122

173 <- 191 0.00118

173 <- 195 0.00183

173 <- 204 0.00227

174 <- 191 -0.00303

174 <- 204 0.00243

174 <- 220 -0.00119

174 <- 321 -0.00107

175 <- 193 -0.00189

175 <- 201 -0.00172

175 <- 202 0.00225

175 <- 205 0.00125

176 <- 197 0.00313

176 <- 198 -0.00114

181 <- 196 -0.00242

181 <- 199 0.00125

181 <- 234 -0.00207

182 <- 192 0.00140

182 <- 196 -0.00698

182 <- 199 0.00115

182 <- 221 -0.00118

183 <- 197 0.00309

183 <- 198 0.00249

183 <- 226 0.00141

183 <- 231 -0.00151

184 <- 193 -0.00675

184 <- 194 0.00659

184 <- 207 0.00134

185 <- 191 -0.00150

185 <- 195 -0.00262

185 <- 200 -0.00152

186 <- 192 -0.00435

186 <- 196 0.00552

186 <- 199 0.00245

186 <- 203 0.00172

186 <- 221 -0.00125

187 <- 193 0.00486

187 <- 194 0.00387

188 <- 197 -0.00392

188 <- 198 0.00118

188 <- 206 -0.00156

188 <- 226 0.00148

189 <- 191 -0.00910

189 <- 195 0.00254

189 <- 200 0.00109

189 <- 220 -0.00182

190 <- 191 0.00974

190 <- 195 0.00865

190 <- 200 -0.00563

190 <- 220 0.00284

Excited State 9: Singlet-B1 2.9424 eV 421.37 nm f=0.3284 <S\*\*2>=0.000

108 -> 252 0.00101

112 -> 240 -0.00101

114 -> 210 -0.00100

114 -> 213 0.00108

116 -> 211 0.00141

118 -> 211 0.00121

118 -> 217 -0.00104

119 -> 213 -0.00110

119 -> 238 0.00117

120 -> 241 -0.00124

122 -> 191 -0.00170

123 -> 216 -0.00133

123 -> 227 0.00127

124 -> 210 0.00128

125 -> 214 -0.00206

125 -> 219 0.00151

125 -> 230 0.00108

125 -> 251 -0.00108

126 -> 209 0.00150

126 -> 216 -0.00208

130 -> 193 -0.00192

132 -> 240 0.00131

132 -> 258 0.00124

133 -> 211 -0.00122

134 -> 211 0.00111

137 -> 211 -0.00107

138 -> 237 -0.00112

138 -> 241 -0.00119

138 -> 251 0.00101

139 -> 210 0.00108

139 -> 297 0.00109

140 -> 222 -0.00128

140 -> 240 -0.00142

141 -> 191 0.00237

141 -> 195 -0.00184

141 -> 204 -0.00102

142 -> 222 0.00119

142 -> 240 0.00116

144 -> 219 -0.00155

144 -> 224 0.00174

144 -> 251 -0.00115

147 -> 194 0.00108

147 -> 207 -0.00102

147 -> 299 0.00101

148 -> 197 -0.00117

148 -> 198 0.00111

150 -> 192 -0.00232

150 -> 196 -0.00249

150 -> 203 -0.00114

151 -> 191 0.00444

152 -> 235 0.00113

152 -> 253 0.00153

153 -> 225 -0.00106

153 -> 232 -0.00125

153 -> 250 0.00140

153 -> 286 0.00125

153 -> 287 -0.00100

153 -> 297 -0.00110

155 -> 228 -0.00161

155 -> 235 0.00101

156 -> 236 -0.00120

156 -> 258 0.00107

156 -> 274 0.00102

157 -> 230 0.00127

157 -> 237 -0.00137

157 -> 256 -0.00107

157 -> 260 0.00135

159 -> 274 0.00113

160 -> 193 -0.00229

160 -> 194 -0.00543

160 -> 201 -0.00174

160 -> 205 0.00208

161 -> 197 0.00452

162 -> 210 0.00109

162 -> 218 0.00121

162 -> 225 0.00190

164 -> 223 0.00179

164 -> 228 0.00124

165 -> 208 0.00117

165 -> 217 0.00116

165 -> 223 0.00131

166 -> 195 -0.00376

166 -> 200 0.00137

166 -> 204 -0.00158

166 -> 220 0.00135

167 -> 205 0.00108

167 -> 218 -0.00131

169 -> 191 0.00165

169 -> 195 0.00283

169 -> 204 0.00258

170 -> 197 -0.00556

170 -> 206 -0.00364

171 -> 194 -0.00111

171 -> 207 -0.00513

172 -> 265 -0.00186

173 -> 196 -0.00365

173 -> 199 0.00185

173 -> 203 -0.00340

173 -> 221 0.00252

173 -> 234 -0.00155

174 -> 192 0.01919

174 -> 196 0.00358

174 -> 199 0.00407

174 -> 203 0.00575

174 -> 221 -0.00176

174 -> 320 -0.00142

175 -> 197 0.00533

175 -> 198 0.00361

175 -> 206 -0.00136

175 -> 315 0.00117

175 -> 322 -0.00102

176 -> 193 0.00324

176 -> 194 -0.00183

176 -> 201 -0.00318

176 -> 202 -0.00252

176 -> 205 0.00225

176 -> 207 -0.00266

176 -> 229 -0.00139

176 -> 232 -0.00118

177 -> 214 0.00126

178 -> 218 -0.00100

178 -> 238 0.00114

178 -> 252 0.00113

179 -> 191 0.00283

179 -> 253 0.00112

180 -> 192 -0.00975

180 -> 199 -0.00116

180 -> 216 0.00121

180 -> 240 0.00106

181 -> 191 0.01920

181 -> 195 -0.00953

181 -> 200 0.00264

181 -> 220 0.00146

181 -> 233 -0.00313

182 -> 191 -0.00970

182 -> 195 -0.02566

182 -> 200 0.00261

182 -> 204 -0.00156

182 -> 220 -0.00179

183 -> 193 0.02640

183 -> 194 0.02764

183 -> 201 0.00118

183 -> 205 -0.00174

183 -> 207 -0.00348

184 -> 197 0.00756

184 -> 198 -0.00620

184 -> 206 -0.00178

184 -> 226 -0.00258

184 -> 231 -0.00248

185 -> 192 -0.00756

185 -> 196 -0.00458

185 -> 199 0.00897

185 -> 203 0.00138

185 -> 221 -0.00225

185 -> 234 0.00131

185 -> 248 0.00111

186 -> 191 0.05410

186 -> 195 -0.02158

186 -> 200 -0.00529

186 -> 204 -0.00388

186 -> 220 0.00257

186 -> 233 0.00119

187 -> 197 0.02853

187 -> 198 0.00787

187 -> 231 0.00113

187 -> 247 -0.00148

187 -> 354 0.00130

188 -> 193 0.01898

188 -> 194 -0.00264

188 -> 202 -0.00493

188 -> 207 0.00742

188 -> 229 0.00131

188 -> 232 0.00117

188 -> 255 0.00123

189 -> 192 0.69391

189 -> 196 0.01073

189 -> 199 0.00356

189 -> 221 -0.00302

189 -> 248 -0.00126

189 -> 349 -0.00107

190 -> 192 0.01397

190 -> 196 0.09951

190 -> 199 0.00635

190 -> 221 -0.00139

190 -> 234 -0.00105

125 <- 214 -0.00128

126 <- 216 -0.00130

130 <- 193 -0.00110

141 <- 191 0.00142

141 <- 195 -0.00121

144 <- 224 0.00109

150 <- 192 -0.00260

150 <- 196 -0.00126

151 <- 191 0.00245

152 <- 253 0.00104

160 <- 193 -0.00189

160 <- 194 -0.00273

160 <- 201 -0.00116

160 <- 205 0.00123

161 <- 197 0.00208

162 <- 225 0.00108

164 <- 223 0.00102

166 <- 195 -0.00214

166 <- 200 0.00103

166 <- 204 -0.00101

169 <- 191 0.00170

169 <- 195 0.00150

169 <- 204 0.00151

170 <- 206 -0.00116

171 <- 207 -0.00212

172 <- 265 -0.00122

173 <- 192 -0.00118

173 <- 196 -0.00183

173 <- 203 -0.00227

174 <- 192 -0.00303

174 <- 203 0.00243

174 <- 221 -0.00119

174 <- 320 -0.00107

175 <- 197 0.00313

175 <- 198 0.00114

176 <- 193 0.00189

176 <- 201 -0.00172

176 <- 202 -0.00225

176 <- 205 0.00125

181 <- 195 -0.00242

181 <- 200 0.00125

181 <- 233 -0.00207

182 <- 191 0.00140

182 <- 195 -0.00698

182 <- 200 0.00115

182 <- 220 -0.00118

183 <- 193 0.00675

183 <- 194 0.00659

183 <- 207 -0.00134

184 <- 197 0.00309

184 <- 198 -0.00249

184 <- 226 -0.00141

184 <- 231 -0.00151

185 <- 192 0.00150

185 <- 196 0.00262

185 <- 199 0.00152

186 <- 191 0.00435

186 <- 195 -0.00552

186 <- 200 -0.00245

186 <- 204 -0.00172

186 <- 220 0.00125

187 <- 197 -0.00392

187 <- 198 -0.00118

187 <- 206 -0.00156

187 <- 226 -0.00148

188 <- 193 -0.00486

188 <- 194 0.00387

189 <- 192 -0.00910

189 <- 196 0.00254

189 <- 199 0.00109

189 <- 221 -0.00182

190 <- 192 -0.00974

190 <- 196 -0.00865

190 <- 199 0.00563

190 <- 221 -0.00284

Excited State 10: Singlet-A1 2.9478 eV 420.60 nm f=0.0000 <S\*\*2>=0.000

97 -> 225 0.00107

101 -> 260 0.00102

109 -> 238 0.00116

113 -> 212 0.00122

114 -> 211 0.00122

116 -> 213 0.00146

118 -> 218 0.00149

122 -> 193 -0.00392

122 -> 202 0.00195

122 -> 207 -0.00102

123 -> 219 -0.00154

123 -> 230 -0.00122

124 -> 217 -0.00157

125 -> 216 0.00157

126 -> 214 0.00232

128 -> 192 0.00153

128 -> 196 -0.00115

129 -> 191 0.00153

129 -> 195 -0.00116

130 -> 191 -0.00286

130 -> 195 0.00234

130 -> 204 0.00114

131 -> 192 0.00286

131 -> 196 -0.00234

131 -> 203 -0.00114

132 -> 241 0.00153

132 -> 260 0.00115

133 -> 213 -0.00123

134 -> 210 -0.00121

135 -> 288 -0.00115

136 -> 289 0.00115

137 -> 287 0.00116

138 -> 240 -0.00103

139 -> 239 -0.00103

140 -> 224 -0.00148

140 -> 237 -0.00148

141 -> 194 0.00316

141 -> 205 -0.00220

142 -> 219 -0.00161

142 -> 251 -0.00139

143 -> 217 -0.00102

143 -> 223 0.00121

144 -> 216 -0.00102

144 -> 222 0.00121

145 -> 224 0.00129

146 -> 207 0.00270

147 -> 191 -0.00162

147 -> 204 -0.00110

147 -> 220 0.00143

148 -> 192 0.00161

148 -> 203 0.00111

148 -> 221 -0.00143

150 -> 198 0.00131

151 -> 194 0.00147

152 -> 225 0.00101

152 -> 286 -0.00127

153 -> 228 0.00127

153 -> 253 -0.00109

154 -> 227 -0.00127

154 -> 254 0.00109

155 -> 229 -0.00113

155 -> 232 0.00120

155 -> 250 -0.00148

156 -> 230 0.00127

156 -> 260 0.00145

157 -> 258 0.00116

158 -> 257 -0.00116

159 -> 237 0.00119

159 -> 256 0.00118

160 -> 195 0.00232

160 -> 200 0.00134

160 -> 204 0.00156

160 -> 220 -0.00246

160 -> 233 0.00146

161 -> 196 0.00232

161 -> 199 0.00134

161 -> 203 0.00156

161 -> 221 -0.00246

161 -> 234 0.00146

162 -> 208 -0.00107

162 -> 223 -0.00124

162 -> 228 -0.00101

163 -> 209 0.00107

163 -> 222 -0.00124

163 -> 227 -0.00101

164 -> 225 -0.00209

165 -> 210 -0.00116

165 -> 215 -0.00104

165 -> 218 -0.00131

165 -> 250 -0.00114

166 -> 193 0.00105

166 -> 207 -0.00530

169 -> 194 -0.00273

169 -> 201 -0.00192

169 -> 229 -0.00179

169 -> 232 -0.00163

169 -> 255 -0.00137

170 -> 192 0.00554

170 -> 196 0.00151

170 -> 203 0.00179

171 -> 191 -0.00555

171 -> 195 -0.00151

171 -> 204 -0.00178

172 -> 238 0.00104

172 -> 252 0.00221

173 -> 197 -0.00438

173 -> 206 -0.00506

173 -> 231 -0.00167

173 -> 247 0.00136

173 -> 315 0.00119

174 -> 198 0.00493

174 -> 322 -0.00117

175 -> 192 0.01292

175 -> 199 0.00641

175 -> 203 0.00163

176 -> 191 -0.01291

176 -> 200 -0.00640

176 -> 204 -0.00163

177 -> 192 0.00418

177 -> 199 0.00144

177 -> 244 0.00124

177 -> 288 -0.00104

178 -> 191 0.00418

178 -> 200 0.00144

178 -> 245 -0.00124

178 -> 289 0.00104

179 -> 194 0.00219

179 -> 201 0.00323

179 -> 205 0.00484

179 -> 215 0.00432

179 -> 218 -0.00171

179 -> 243 0.00276

179 -> 271 0.00118

179 -> 287 0.00105

179 -> 293 0.00127

179 -> 334 -0.00112

179 -> 414 -0.00161

180 -> 251 -0.00167

180 -> 294 -0.00162

180 -> 310 -0.00120

181 -> 193 0.01602

182 -> 193 0.02005

182 -> 202 0.00334

182 -> 207 -0.00658

183 -> 191 0.02882

183 -> 195 -0.02528

183 -> 200 -0.00126

183 -> 204 -0.00116

183 -> 220 0.00270

183 -> 233 -0.00194

184 -> 192 -0.02881

184 -> 196 0.02533

184 -> 199 0.00127

184 -> 203 0.00116

184 -> 221 -0.00269

184 -> 234 0.00194

185 -> 197 0.03663

185 -> 206 0.00520

185 -> 231 0.00227

185 -> 247 -0.00188

186 -> 194 0.03015

186 -> 205 -0.00124

186 -> 229 0.00232

186 -> 232 0.00204

186 -> 255 0.00140

187 -> 192 -0.48622

187 -> 196 -0.00965

187 -> 199 -0.00361

187 -> 234 0.00195

187 -> 248 0.00203

188 -> 191 0.48642

188 -> 195 0.00969

188 -> 200 0.00361

188 -> 233 -0.00195

188 -> 249 -0.00203

189 -> 198 -0.00499

189 -> 246 -0.00133

189 -> 354 -0.00122

190 -> 197 0.14216

190 -> 206 0.00444

190 -> 231 -0.00124

122 <- 193 -0.00233

122 <- 202 0.00129

126 <- 214 0.00143

130 <- 191 -0.00158

130 <- 195 0.00156

131 <- 192 0.00158

131 <- 196 -0.00156

132 <- 241 0.00102

141 <- 194 0.00226

141 <- 205 -0.00153

146 <- 207 0.00131

151 <- 194 0.00115

155 <- 250 -0.00100

160 <- 191 -0.00105

160 <- 195 0.00214

160 <- 204 0.00121

161 <- 192 -0.00105

161 <- 196 0.00214

161 <- 203 0.00121

164 <- 225 -0.00119

166 <- 193 0.00173

166 <- 207 -0.00239

169 <- 194 -0.00115

169 <- 201 -0.00102

170 <- 192 0.00148

170 <- 221 -0.00132

171 <- 191 -0.00149

171 <- 220 0.00132

172 <- 252 0.00137

173 <- 197 0.00118

173 <- 247 0.00111

174 <- 198 0.00126

174 <- 226 0.00101

174 <- 246 -0.00102

175 <- 192 -0.00265

176 <- 191 0.00265

179 <- 201 0.00123

179 <- 205 0.00184

179 <- 215 0.00200

179 <- 243 0.00151

179 <- 414 -0.00122

180 <- 294 -0.00110

181 <- 193 0.00120

181 <- 202 0.00133

181 <- 207 -0.00205

182 <- 193 0.00707

182 <- 207 -0.00169

183 <- 191 0.00185

183 <- 195 -0.00628

183 <- 200 -0.00118

183 <- 220 0.00155

184 <- 192 -0.00185

184 <- 196 0.00629

184 <- 199 0.00118

184 <- 221 -0.00155

185 <- 231 0.00125

186 <- 194 0.00708

186 <- 229 0.00114

186 <- 232 0.00100

187 <- 192 0.00517

187 <- 199 -0.00141

187 <- 221 0.00123

187 <- 234 0.00129

187 <- 248 0.00111

188 <- 191 -0.00517

188 <- 200 0.00140

188 <- 220 -0.00122

188 <- 233 -0.00129

188 <- 249 -0.00111

189 <- 198 0.00233

189 <- 226 0.00215

189 <- 246 -0.00118

190 <- 197 0.01404

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

Leave Link 914 at Thu Sep 19 01:06:09 2019, MaxMem= 1342177280 cpu: 14038.2

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

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The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.31952 -14.31952 -14.31952 -14.31951 -14.31593

Alpha occ. eigenvalues -- -14.31593 -14.31593 -14.31593 -10.24966 -10.24966

Alpha occ. eigenvalues -- -10.24966 -10.24966 -10.24965 -10.24965 -10.24965

Alpha occ. eigenvalues -- -10.24964 -10.19130 -10.19130 -10.19130 -10.19130

Alpha occ. eigenvalues -- -10.19092 -10.19092 -10.19092 -10.19092 -10.18504

Alpha occ. eigenvalues -- -10.18504 -10.18504 -10.18504 -10.18477 -10.18477

Alpha occ. eigenvalues -- -10.18477 -10.18477 -10.18429 -10.18429 -10.18429

Alpha occ. eigenvalues -- -10.18429 -10.18415 -10.18414 -10.18414 -10.18414

Alpha occ. eigenvalues -- -10.17668 -10.17668 -10.17668 -10.17668 -10.17666

Alpha occ. eigenvalues -- -10.17666 -10.17666 -10.17666 -10.17583 -10.17583

Alpha occ. eigenvalues -- -10.17583 -10.17583 -10.17542 -10.17542 -10.17542

Alpha occ. eigenvalues -- -10.17542 -1.00782 -0.99415 -0.99415 -0.96684

Alpha occ. eigenvalues -- -0.94560 -0.90529 -0.90529 -0.88380 -0.88056

Alpha occ. eigenvalues -- -0.88008 -0.88008 -0.86908 -0.82949 -0.82802

Alpha occ. eigenvalues -- -0.82802 -0.82712 -0.79056 -0.78476 -0.78476

Alpha occ. eigenvalues -- -0.78342 -0.75595 -0.75545 -0.75440 -0.75440

Alpha occ. eigenvalues -- -0.75240 -0.73603 -0.73603 -0.72875 -0.70742

Alpha occ. eigenvalues -- -0.69231 -0.69231 -0.65905 -0.65664 -0.65095

Alpha occ. eigenvalues -- -0.65095 -0.63009 -0.62801 -0.60969 -0.60969

Alpha occ. eigenvalues -- -0.60501 -0.60271 -0.60222 -0.60222 -0.60109

Alpha occ. eigenvalues -- -0.60108 -0.58376 -0.57186 -0.56970 -0.56970

Alpha occ. eigenvalues -- -0.56221 -0.54677 -0.54677 -0.54199 -0.53733

Alpha occ. eigenvalues -- -0.53733 -0.53309 -0.51703 -0.51703 -0.51691

Alpha occ. eigenvalues -- -0.51643 -0.51579 -0.51188 -0.50811 -0.50811

Alpha occ. eigenvalues -- -0.49408 -0.46379 -0.45691 -0.45645 -0.45645

Alpha occ. eigenvalues -- -0.45530 -0.45449 -0.44974 -0.44974 -0.44882

Alpha occ. eigenvalues -- -0.44882 -0.44278 -0.44032 -0.43837 -0.43509

Alpha occ. eigenvalues -- -0.43509 -0.43275 -0.42923 -0.42923 -0.42468

Alpha occ. eigenvalues -- -0.42422 -0.42183 -0.42040 -0.42040 -0.41381

Alpha occ. eigenvalues -- -0.39669 -0.39583 -0.39583 -0.39050 -0.38771

Alpha occ. eigenvalues -- -0.38521 -0.37821 -0.37395 -0.37395 -0.36702

Alpha occ. eigenvalues -- -0.35654 -0.35480 -0.35480 -0.35235 -0.34229

Alpha occ. eigenvalues -- -0.34229 -0.34046 -0.34046 -0.33963 -0.33609

Alpha occ. eigenvalues -- -0.33157 -0.32875 -0.32875 -0.32051 -0.31505

Alpha occ. eigenvalues -- -0.31505 -0.30909 -0.30424 -0.29627 -0.29206

Alpha occ. eigenvalues -- -0.29206 -0.28196 -0.28196 -0.26968 -0.26570

Alpha occ. eigenvalues -- -0.25412 -0.25220 -0.24982 -0.24982 -0.24823

Alpha occ. eigenvalues -- -0.24780 -0.22789 -0.22789 -0.22680 -0.17259

Alpha virt. eigenvalues -- -0.10335 -0.10335 -0.06198 -0.05881 -0.05506

Alpha virt. eigenvalues -- -0.05506 -0.04516 -0.00082 0.00025 0.00025

Alpha virt. eigenvalues -- 0.00680 0.00732 0.01363 0.01363 0.02042

Alpha virt. eigenvalues -- 0.02994 0.04955 0.04980 0.04980 0.05953

Alpha virt. eigenvalues -- 0.06294 0.06294 0.06301 0.06376 0.07025

Alpha virt. eigenvalues -- 0.07353 0.07353 0.07740 0.08364 0.09334

Alpha virt. eigenvalues -- 0.09334 0.09718 0.09718 0.10551 0.10952

Alpha virt. eigenvalues -- 0.11328 0.11682 0.11682 0.12262 0.12352

Alpha virt. eigenvalues -- 0.12355 0.12601 0.13069 0.13069 0.13392

Alpha virt. eigenvalues -- 0.13392 0.14410 0.14682 0.16454 0.16454

Alpha virt. eigenvalues -- 0.17927 0.18286 0.18313 0.18651 0.18651

Alpha virt. eigenvalues -- 0.18820 0.19051 0.19058 0.19058 0.19759

Alpha virt. eigenvalues -- 0.20597 0.21435 0.22204 0.22204 0.22388

Alpha virt. eigenvalues -- 0.23080 0.23162 0.23162 0.24334 0.24549

Alpha virt. eigenvalues -- 0.25424 0.25424 0.26175 0.26237 0.26237

Alpha virt. eigenvalues -- 0.26979 0.27821 0.27821 0.27854 0.28013

Alpha virt. eigenvalues -- 0.28067 0.28128 0.28537 0.28537 0.28855

Alpha virt. eigenvalues -- 0.29185 0.29185 0.29733 0.30535 0.30761

Alpha virt. eigenvalues -- 0.30761 0.30867 0.31152 0.31152 0.31203

Alpha virt. eigenvalues -- 0.31904 0.31918 0.32779 0.32779 0.33328

Alpha virt. eigenvalues -- 0.34653 0.34653 0.35032 0.35185 0.35847

Alpha virt. eigenvalues -- 0.35847 0.36149 0.36591 0.36882 0.37212

Alpha virt. eigenvalues -- 0.37212 0.37355 0.37606 0.38057 0.38057

Alpha virt. eigenvalues -- 0.38142 0.38361 0.38532 0.38532 0.39024

Alpha virt. eigenvalues -- 0.39234 0.39281 0.39281 0.39744 0.39946

Alpha virt. eigenvalues -- 0.40197 0.40245 0.40295 0.40295 0.40866

Alpha virt. eigenvalues -- 0.40866 0.41140 0.41265 0.41700 0.41700

Alpha virt. eigenvalues -- 0.42016 0.42680 0.42880 0.42880 0.43099

Alpha virt. eigenvalues -- 0.43221 0.43221 0.43299 0.43427 0.43529

Alpha virt. eigenvalues -- 0.43671 0.43671 0.43681 0.44063 0.44091

Alpha virt. eigenvalues -- 0.44506 0.44506 0.44734 0.44882 0.45099

Alpha virt. eigenvalues -- 0.45099 0.45373 0.46204 0.46231 0.46231

Alpha virt. eigenvalues -- 0.46468 0.46468 0.46675 0.46706 0.47134

Alpha virt. eigenvalues -- 0.47134 0.47315 0.47571 0.47645 0.47645

Alpha virt. eigenvalues -- 0.48204 0.48468 0.48795 0.48968 0.49341

Alpha virt. eigenvalues -- 0.49341 0.49721 0.50425 0.50782 0.50871

Alpha virt. eigenvalues -- 0.50871 0.51116 0.51562 0.51562 0.52239

Alpha virt. eigenvalues -- 0.52240 0.53216 0.53384 0.53384 0.53425

Alpha virt. eigenvalues -- 0.53759 0.53866 0.54683 0.54977 0.55679

Alpha virt. eigenvalues -- 0.55679 0.56454 0.56454 0.56915 0.58116

Alpha virt. eigenvalues -- 0.58116 0.58914 0.58967 0.59474 0.60241

Alpha virt. eigenvalues -- 0.60241 0.60730 0.60884 0.60884 0.61229

Alpha virt. eigenvalues -- 0.61334 0.61727 0.61838 0.61838 0.62251

Alpha virt. eigenvalues -- 0.62395 0.62688 0.62688 0.62979 0.63021

Alpha virt. eigenvalues -- 0.63223 0.63223 0.63522 0.63598 0.64371

Alpha virt. eigenvalues -- 0.64452 0.64515 0.64515 0.65608 0.65608

Alpha virt. eigenvalues -- 0.65894 0.66329 0.67393 0.67648 0.67648

Alpha virt. eigenvalues -- 0.68147 0.68260 0.68463 0.68570 0.68570

Alpha virt. eigenvalues -- 0.68987 0.69378 0.69378 0.69455 0.70002

Alpha virt. eigenvalues -- 0.70002 0.70672 0.70672 0.70991 0.72359

Alpha virt. eigenvalues -- 0.72959 0.72960 0.73181 0.73293 0.73407

Alpha virt. eigenvalues -- 0.73407 0.74017 0.74674 0.74837 0.75421

Alpha virt. eigenvalues -- 0.75421 0.76028 0.76435 0.76536 0.76710

Alpha virt. eigenvalues -- 0.76710 0.78410 0.78639 0.78720 0.78997

Alpha virt. eigenvalues -- 0.78997 0.79490 0.79490 0.79851 0.80257

Alpha virt. eigenvalues -- 0.80432 0.80432 0.80546 0.80661 0.81394

Alpha virt. eigenvalues -- 0.81625 0.81625 0.82108 0.82368 0.82600

Alpha virt. eigenvalues -- 0.82914 0.82914 0.84192 0.84302 0.84302

Alpha virt. eigenvalues -- 0.85017 0.85171 0.85385 0.85385 0.85827

Alpha virt. eigenvalues -- 0.86155 0.87762 0.87785 0.88041 0.88041

Alpha virt. eigenvalues -- 0.88664 0.88664 0.89966 0.91836 0.91836

Alpha virt. eigenvalues -- 0.92146 0.92862 0.92862 0.93573 0.94542

Alpha virt. eigenvalues -- 0.94847 0.94847 0.95988 0.96024 0.96396

Alpha virt. eigenvalues -- 0.97156 0.97311 0.97311 0.97544 0.97750

Alpha virt. eigenvalues -- 0.97836 0.98200 0.98200 0.98598 0.98715

Alpha virt. eigenvalues -- 0.98715 0.99712 0.99712 0.99790 1.00335

Alpha virt. eigenvalues -- 1.01401 1.02164 1.02344 1.02685 1.02685

Alpha virt. eigenvalues -- 1.03582 1.03960 1.03960 1.05403 1.05563

Alpha virt. eigenvalues -- 1.06382 1.06382 1.07102 1.07102 1.07318

Alpha virt. eigenvalues -- 1.09000 1.09995 1.10031 1.10031 1.10335

Alpha virt. eigenvalues -- 1.10617 1.11232 1.11232 1.11369 1.11503

Alpha virt. eigenvalues -- 1.11610 1.11610 1.12371 1.12606 1.12611

Alpha virt. eigenvalues -- 1.12640 1.12640 1.13727 1.14152 1.14195

Alpha virt. eigenvalues -- 1.14722 1.14722 1.16652 1.16652 1.16686

Alpha virt. eigenvalues -- 1.17184 1.17184 1.17366 1.17858 1.18387

Alpha virt. eigenvalues -- 1.19032 1.19032 1.19653 1.20824 1.21810

Alpha virt. eigenvalues -- 1.21810 1.21821 1.21825 1.21945 1.22533

Alpha virt. eigenvalues -- 1.22630 1.22630 1.23306 1.24723 1.24723

Alpha virt. eigenvalues -- 1.25633 1.25633 1.25880 1.26660 1.26682

Alpha virt. eigenvalues -- 1.27425 1.27425 1.27813 1.27876 1.28567

Alpha virt. eigenvalues -- 1.29235 1.29728 1.30400 1.30515 1.30515

Alpha virt. eigenvalues -- 1.33426 1.33427 1.34481 1.34875 1.35389

Alpha virt. eigenvalues -- 1.35389 1.36231 1.37787 1.38626 1.38997

Alpha virt. eigenvalues -- 1.39330 1.39330 1.40125 1.40126 1.40466

Alpha virt. eigenvalues -- 1.42627 1.42733 1.42733 1.44672 1.44744

Alpha virt. eigenvalues -- 1.44821 1.44821 1.44959 1.45833 1.45833

Alpha virt. eigenvalues -- 1.46315 1.47276 1.48626 1.48626 1.48987

Alpha virt. eigenvalues -- 1.51615 1.51616 1.51654 1.51837 1.51837

Alpha virt. eigenvalues -- 1.51931 1.51991 1.52101 1.52219 1.52372

Alpha virt. eigenvalues -- 1.52372 1.52740 1.53125 1.53125 1.53136

Alpha virt. eigenvalues -- 1.53299 1.54342 1.54395 1.54395 1.55157

Alpha virt. eigenvalues -- 1.56293 1.56743 1.56743 1.57850 1.58259

Alpha virt. eigenvalues -- 1.60975 1.60975 1.64285 1.64576 1.64920

Alpha virt. eigenvalues -- 1.65089 1.65089 1.65328 1.67001 1.68320

Alpha virt. eigenvalues -- 1.68320 1.69567 1.69581 1.69581 1.70892

Alpha virt. eigenvalues -- 1.71230 1.71230 1.71962 1.72232 1.72589

Alpha virt. eigenvalues -- 1.73560 1.74238 1.74238 1.75526 1.75634

Alpha virt. eigenvalues -- 1.77028 1.77028 1.77612 1.78085 1.78086

Alpha virt. eigenvalues -- 1.78087 1.79315 1.80151 1.80151 1.81282

Alpha virt. eigenvalues -- 1.82017 1.82146 1.82210 1.82210 1.82760

Alpha virt. eigenvalues -- 1.83096 1.83097 1.83686 1.84782 1.84782

Alpha virt. eigenvalues -- 1.86212 1.86674 1.86688 1.86688 1.87254

Alpha virt. eigenvalues -- 1.87330 1.88146 1.88750 1.88750 1.88955

Alpha virt. eigenvalues -- 1.89322 1.89645 1.89645 1.90115 1.90547

Alpha virt. eigenvalues -- 1.91631 1.91660 1.91660 1.92152 1.92461

Alpha virt. eigenvalues -- 1.92461 1.92526 1.92655 1.92655 1.92675

Alpha virt. eigenvalues -- 1.92794 1.94304 1.94742 1.94924 1.95112

Alpha virt. eigenvalues -- 1.95112 1.95284 1.95284 1.95752 1.96607

Alpha virt. eigenvalues -- 1.96607 1.96622 1.97099 1.97361 1.97693

Alpha virt. eigenvalues -- 1.97693 1.98114 1.99514 1.99853 1.99853

Alpha virt. eigenvalues -- 2.02267 2.02695 2.04092 2.04788 2.04788

Alpha virt. eigenvalues -- 2.05118 2.07386 2.08441 2.08441 2.09649

Alpha virt. eigenvalues -- 2.12307 2.13202 2.13202 2.15224 2.15224

Alpha virt. eigenvalues -- 2.15545 2.15843 2.18731 2.18731 2.18958

Alpha virt. eigenvalues -- 2.19812 2.21385 2.21385 2.21869 2.21938

Alpha virt. eigenvalues -- 2.22310 2.22310 2.22352 2.22540 2.22856

Alpha virt. eigenvalues -- 2.24463 2.24835 2.24835 2.24986 2.26298

Alpha virt. eigenvalues -- 2.26442 2.26442 2.27605 2.27870 2.28342

Alpha virt. eigenvalues -- 2.28342 2.30072 2.31424 2.31616 2.31776

Alpha virt. eigenvalues -- 2.31776 2.31890 2.32430 2.33920 2.33920

Alpha virt. eigenvalues -- 2.35025 2.35025 2.35054 2.35350 2.36246

Alpha virt. eigenvalues -- 2.36503 2.36503 2.38606 2.39832 2.39833

Alpha virt. eigenvalues -- 2.40660 2.42884 2.43548 2.44129 2.44692

Alpha virt. eigenvalues -- 2.44692 2.45583 2.45583 2.45649 2.46500

Alpha virt. eigenvalues -- 2.47715 2.49965 2.49965 2.51306 2.51898

Alpha virt. eigenvalues -- 2.51898 2.52492 2.53088 2.53166 2.53493

Alpha virt. eigenvalues -- 2.53493 2.54048 2.55194 2.55194 2.55447

Alpha virt. eigenvalues -- 2.56041 2.56041 2.56099 2.56194 2.57098

Alpha virt. eigenvalues -- 2.57574 2.57574 2.57867 2.59006 2.61029

Alpha virt. eigenvalues -- 2.63201 2.65008 2.65008 2.65208 2.65208

Alpha virt. eigenvalues -- 2.65697 2.68119 2.68831 2.69586 2.69726

Alpha virt. eigenvalues -- 2.69726 2.70965 2.70965 2.71226 2.71438

Alpha virt. eigenvalues -- 2.72151 2.72151 2.72647 2.73624 2.73678

Alpha virt. eigenvalues -- 2.73980 2.74016 2.74058 2.74058 2.74595

Alpha virt. eigenvalues -- 2.74664 2.75448 2.75449 2.75861 2.75861

Alpha virt. eigenvalues -- 2.78157 2.80250 2.80740 2.80740 2.80930

Alpha virt. eigenvalues -- 2.81689 2.82380 2.82380 2.82784 2.82956

Alpha virt. eigenvalues -- 2.82957 2.83735 2.84999 2.86527 2.86831

Alpha virt. eigenvalues -- 2.86831 2.86941 2.87640 2.87640 2.87842

Alpha virt. eigenvalues -- 2.88042 2.88820 2.89590 2.89590 2.89642

Alpha virt. eigenvalues -- 2.91138 2.93056 2.93056 2.93823 2.93937

Alpha virt. eigenvalues -- 2.96939 2.96939 2.98990 3.02520 3.03218

Alpha virt. eigenvalues -- 3.03218 3.03997 3.04182 3.05040 3.05576

Alpha virt. eigenvalues -- 3.05576 3.07640 3.09302 3.09302 3.15071

Alpha virt. eigenvalues -- 3.15628 3.15628 3.15914 3.16857 3.17823

Alpha virt. eigenvalues -- 3.17823 3.18973 3.19378 3.20410 3.20453

Alpha virt. eigenvalues -- 3.20453 3.20543 3.21429 3.21490 3.21490

Alpha virt. eigenvalues -- 3.22520 3.23171 3.23642 3.24560 3.24560

Alpha virt. eigenvalues -- 3.26333 3.26919 3.27350 3.27350 3.28367

Alpha virt. eigenvalues -- 3.28564 3.28564 3.28652 3.29131 3.29268

Alpha virt. eigenvalues -- 3.29268 3.29318 3.31630 3.31945 3.31945

Alpha virt. eigenvalues -- 3.32475 3.32492 3.33917 3.33917 3.34024

Alpha virt. eigenvalues -- 3.34786 3.35114 3.35114 3.37586 3.39907

Alpha virt. eigenvalues -- 3.41283 3.41283 3.42165 3.42249 3.42918

Alpha virt. eigenvalues -- 3.42918 3.43685 3.46785 3.47140 3.47140

Alpha virt. eigenvalues -- 3.47758 3.51636 3.52115 3.52115 3.53003

Alpha virt. eigenvalues -- 3.53195 3.53195 3.53299 3.53378 3.55311

Alpha virt. eigenvalues -- 3.60086 3.60086 3.62491 3.62754 3.63168

Alpha virt. eigenvalues -- 3.63168 3.70490 3.71011 3.71011 3.71799

Alpha virt. eigenvalues -- 3.75101 3.75726 3.75727 3.76843 3.82954

Alpha virt. eigenvalues -- 3.83514 3.83700 3.83700 3.87439 3.88297

Alpha virt. eigenvalues -- 3.88670 3.89369 3.89369 3.89717 3.90055

Alpha virt. eigenvalues -- 3.90055 3.91022 4.00805 4.01153 4.01153

Alpha virt. eigenvalues -- 4.02326 4.03151 4.03584 4.03584 4.06130

Alpha virt. eigenvalues -- 4.11841 4.13033 4.13033 4.20896 4.24176

Alpha virt. eigenvalues -- 4.28844 4.28844 4.38992 4.40996 4.42965

Alpha virt. eigenvalues -- 4.44978 4.44978 4.47195 4.53231 4.53231

Alpha virt. eigenvalues -- 4.54457 4.75875 4.75875 4.75880 4.75900

Alpha virt. eigenvalues -- 4.79029 4.79094 4.79094 4.79233 5.12469

Alpha virt. eigenvalues -- 5.12469 5.13467 5.16221 5.23133 5.37058

Alpha virt. eigenvalues -- 5.37058 5.52396 7.82539 7.87339 7.87339

Alpha virt. eigenvalues -- 7.88520 8.10137 11.10218 23.20698 23.22355

Alpha virt. eigenvalues -- 23.22355 23.23287 23.56491 23.58438 23.58438

Alpha virt. eigenvalues -- 23.59415 23.72291 23.72492 23.72492 23.72670

Alpha virt. eigenvalues -- 23.81416 23.81477 23.81790 23.81790 23.82217

Alpha virt. eigenvalues -- 23.82982 23.82982 23.84834 23.88936 23.89861

Alpha virt. eigenvalues -- 23.89861 23.90535 23.92355 23.92506 23.92524

Alpha virt. eigenvalues -- 23.92524 23.98130 23.98241 23.98241 23.98437

Alpha virt. eigenvalues -- 24.06942 24.06949 24.06949 24.06961 24.10069

Alpha virt. eigenvalues -- 24.10069 24.10115 24.10118 24.14086 24.14171

Alpha virt. eigenvalues -- 24.14171 24.14257 24.14478 24.14646 24.14646

Alpha virt. eigenvalues -- 24.15189 35.56578 35.60124 35.60124 35.61462

Alpha virt. eigenvalues -- 35.69267 35.70143 35.70143 35.70242

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C 0.386683

2 N -0.645418

3 C 0.386683

4 C -0.072858

5 C -0.072858

6 N -0.403973

7 C 0.386682

8 N -0.645417

9 C 0.386682

10 C -0.072857

11 C -0.072857

12 N -0.403973

13 C -0.072857

14 C -0.072857

15 C 0.386682

16 N -0.645417

17 C 0.386682

18 N -0.403973

19 N -0.645418

20 C 0.386683

21 C -0.072858

22 C -0.072858

23 C 0.386683

24 N -0.403973

25 Zn 1.404122

26 C -0.210552

27 C 0.009122

28 C 0.009122

29 C -0.210552

30 C -0.210552

31 C 0.009122

32 C 0.009122

33 C -0.210552

34 C -0.210552

35 C 0.009122

36 C 0.009122

37 C -0.210552

38 C -0.210552

39 C 0.009122

40 C 0.009122

41 C -0.210552

42 C -0.229471

43 C -0.222402

44 C -0.222402

45 C -0.229471

46 C -0.229471

47 C -0.222402

48 C -0.222402

49 C -0.229471

50 C -0.229471

51 C -0.222402

52 C -0.222402

53 C -0.229471

54 C -0.229471

55 C -0.222402

56 C -0.222402

57 C -0.229471

58 H 0.230376

59 H 0.230376

60 H 0.230376

61 H 0.230376

62 H 0.230376

63 H 0.230376

64 H 0.230376

65 H 0.230376

66 H 0.229879

67 H 0.228402

68 H 0.228402

69 H 0.229879

70 H 0.229879

71 H 0.228402

72 H 0.228402

73 H 0.229879

74 H 0.229879

75 H 0.228402

76 H 0.228402

77 H 0.229879

78 H 0.229879

79 H 0.228402

80 H 0.228402

81 H 0.229879

Sum of Mulliken charges = -0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C 0.386683

2 N -0.645418

3 C 0.386683

4 C -0.072858

5 C -0.072858

6 N -0.403973

7 C 0.386682

8 N -0.645417

9 C 0.386682

10 C -0.072857

11 C -0.072857

12 N -0.403973

13 C -0.072857

14 C -0.072857

15 C 0.386682

16 N -0.645417

17 C 0.386682

18 N -0.403973

19 N -0.645418

20 C 0.386683

21 C -0.072858

22 C -0.072858

23 C 0.386683

24 N -0.403973

25 Zn 1.404122

26 C 0.019824

27 C 0.009122

28 C 0.009122

29 C 0.019824

30 C 0.019824

31 C 0.009122

32 C 0.009122

33 C 0.019824

34 C 0.019824

35 C 0.009122

36 C 0.009122

37 C 0.019824

38 C 0.019824

39 C 0.009122

40 C 0.009122

41 C 0.019824

42 C 0.000408

43 C 0.006000

44 C 0.006000

45 C 0.000408

46 C 0.000409

47 C 0.006000

48 C 0.006000

49 C 0.000409

50 C 0.000408

51 C 0.006000

52 C 0.006000

53 C 0.000408

54 C 0.000409

55 C 0.006000

56 C 0.006000

57 C 0.000409

Electronic spatial extent (au): <R\*\*2>= 50409.6148

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= -0.0000 Z= 2.6053 Tot= 2.6053

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

XX= -268.3099 YY= -268.3103 ZZ= -337.6642

XY= -0.0000 XZ= -0.0000 YZ= 0.0000

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

XX= 23.1183 YY= 23.1179 ZZ= -46.2361

XY= -0.0000 XZ= -0.0000 YZ= 0.0000

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

XXX= -0.0000 YYY= 0.0000 ZZZ= 60.4769 XYY= 0.0000

XXY= -0.0000 XXZ= -40.2036 XZZ= 0.0000 YZZ= 0.0000

YYZ= -40.2213 XYZ= 0.0000

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

XXXX= -28224.7506 YYYY= -28224.7172 ZZZZ= -486.6928 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -10322.7273 XXZZ= -6609.7966 YYZZ= -6609.7506

XXYZ= 0.0000 YYXZ= -0.0000 ZZXY= -0.0000

N-N= 6.888572816868D+03 E-N=-1.931954521448D+04 KE= 2.388757903125D+03

Symmetry A1 KE= 6.742197496188D+02

Symmetry A2 KE= 5.331437604629D+02

Symmetry B1 KE= 5.906971971451D+02

Symmetry B2 KE= 5.906971958986D+02

Leave Link 601 at Thu Sep 19 01:06:36 2019, MaxMem= 1342177280 cpu: 46.3

(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\C48H24N8Zn1

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

nt=dmso,smd) empiricaldispersion=gd3bj IOp(9/40=3)\\ZnNPC0td\\0,1\C,0,

1.122077,2.793021,0.172784\N,0,0.,2.020361,0.259821\C,0,-1.122077,2.79

3021,0.172784\C,0,-0.714524,4.194635,0.051468\C,0,0.714524,4.194635,0.

051468\N,0,-2.389506,2.389505,0.154613\C,0,-2.793023,1.122077,0.172801

\N,0,-2.020362,0.,0.259826\C,0,-2.793023,-1.122077,0.172801\C,0,-4.194

641,-0.714524,0.051526\C,0,-4.194641,0.714524,0.051526\N,0,2.389506,2.

389505,0.154613\C,0,4.194641,0.714524,0.051526\C,0,4.194641,-0.714524,

0.051526\C,0,2.793023,-1.122077,0.172801\N,0,2.020362,0.,0.259826\C,0,

2.793023,1.122077,0.172801\N,0,2.389506,-2.389505,0.154613\N,0,0.,-2.0

20361,0.259821\C,0,1.122077,-2.793021,0.172784\C,0,0.714524,-4.194635,

0.051468\C,0,-0.714524,-4.194635,0.051468\C,0,-1.122077,-2.793021,0.17

2784\N,0,-2.389506,-2.389505,0.154613\Zn,0,0.,0.,0.777528\C,0,5.363492

,1.427454,-0.054616\C,0,6.58861,0.72073,-0.156377\C,0,6.58861,-0.72073

,-0.156377\C,0,5.363492,-1.427454,-0.054616\C,0,-1.427454,-5.363483,-0

.054708\C,0,-0.72073,-6.588598,-0.156501\C,0,0.72073,-6.588598,-0.1565

01\C,0,1.427454,-5.363483,-0.054708\C,0,-5.363492,1.427454,-0.054616\C

,0,-6.58861,0.72073,-0.156377\C,0,-6.58861,-0.72073,-0.156377\C,0,-5.3

63492,-1.427454,-0.054616\C,0,1.427454,5.363483,-0.054708\C,0,0.72073,

6.588598,-0.156501\C,0,-0.72073,6.588598,-0.156501\C,0,-1.427454,5.363

483,-0.054708\C,0,1.402412,-7.830417,-0.258961\C,0,0.708074,-9.011507,

-0.356784\C,0,-0.708074,-9.011507,-0.356784\C,0,-1.402412,-7.830417,-0

.258961\C,0,7.830431,-1.402412,-0.258803\C,0,9.011524,-0.708074,-0.356

593\C,0,9.011524,0.708074,-0.356593\C,0,7.830431,1.402412,-0.258803\C,

0,-1.402412,7.830417,-0.258961\C,0,-0.708074,9.011507,-0.356784\C,0,0.

708074,9.011507,-0.356784\C,0,1.402412,7.830417,-0.258961\C,0,-7.83043

1,-1.402412,-0.258803\C,0,-9.011524,-0.708074,-0.356593\C,0,-9.011524,

0.708074,-0.356593\C,0,-7.830431,1.402412,-0.258803\H,0,5.364985,2.512

421,-0.058211\H,0,5.364985,-2.512421,-0.058211\H,0,-2.512421,-5.364975

,-0.058303\H,0,2.512421,-5.364975,-0.058303\H,0,-5.364985,2.512421,-0.

058211\H,0,-5.364985,-2.512421,-0.058211\H,0,2.512421,5.364975,-0.0583

03\H,0,-2.512421,5.364975,-0.058303\H,0,2.487843,-7.828541,-0.258814\H

,0,1.243262,-9.951788,-0.435088\H,0,-1.243262,-9.951788,-0.435088\H,0,

-2.487843,-7.828541,-0.258814\H,0,7.828556,-2.487843,-0.258655\H,0,9.9

51808,-1.243262,-0.43487\H,0,9.951808,1.243262,-0.43487\H,0,7.828556,2

.487843,-0.258655\H,0,-2.487843,7.828541,-0.258814\H,0,-1.243262,9.951

788,-0.435088\H,0,1.243262,9.951788,-0.435088\H,0,2.487843,7.828541,-0

.258814\H,0,-7.828556,-2.487843,-0.258655\H,0,-9.951808,-1.243262,-0.4

3487\H,0,-9.951808,1.243262,-0.43487\H,0,-7.828556,2.487843,-0.258655\

\Version=ES64L-G09RevE.01\State=1-A1\HF=-2348.1645354\RMSD=5.058e-09\P

G=C02V [C2(Zn1),SGV(N2),SGV'(N2),X(C48H24N4)]\\@

THE SECRET OF SUCCESS IN LIFE IS TO EAT WHAT YOU LIKE, AND LET THE FOOD

FIGHT IT OUT INSIDE YOU. -- FROM A FORTUNE COOKIE

Job cpu time: 0 days 4 hours 36 minutes 47.4 seconds.

File lengths (MBytes): RWF= 4517 Int= 0 D2E= 0 Chk= 459 Scr= 1

Normal termination of Gaussian 09 at Thu Sep 19 01:07:17 2019.