Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-21419.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 21435.

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

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

Cite this work as:

Gaussian 09, Revision D.01,

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

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

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

Gaussian 09: ES64L-G09RevD.01 24-Apr-2013

5-Sep-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%mem=10GB

%chk=ZnTPP0td.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 5 21:44:32 2019, MaxMem= 1342177280 cpu: 0.8

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

--------

ZnTPP0td

--------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C -0.68148 4.26916 0.16409

C -1.11054 2.89013 0.0355

N 0. 2.09053 -0.02746

C 1.11054 2.89013 0.0355

C 0.68148 4.26916 0.16409

C 2.45218 2.45218 0.

C 2.89013 1.11054 -0.0355

N 2.09053 0. 0.02746

C 2.89013 -1.11054 -0.0355

C 4.26916 -0.68148 -0.16409

C 4.26916 0.68148 -0.16409

C -2.45218 2.45218 0.

C -2.89013 1.11054 -0.0355

C -4.26916 0.68148 -0.16409

C -4.26916 -0.68148 -0.16409

C -2.89013 -1.11054 -0.0355

N -2.09053 0. 0.02746

C -2.45218 -2.45218 0.

C -1.11054 -2.89013 0.0355

C -0.68148 -4.26916 0.16409

C 0.68148 -4.26916 0.16409

C 1.11054 -2.89013 0.0355

N 0. -2.09053 -0.02746

C 2.45218 -2.45218 0.

C 3.50824 3.50824 0.

C 3.62136 4.40504 -1.06967

C 4.60749 5.38875 -1.07114

C 5.49381 5.49381 0.

C 5.38875 4.60749 1.07114

C 4.40504 3.62136 1.06967

C -5.49381 5.49381 0.

C -4.60749 5.38875 -1.07114

C -3.62136 4.40504 -1.06967

C -3.50824 3.50824 0.

C -4.40504 3.62136 1.06967

C -5.38875 4.60749 1.07114

C 3.50824 -3.50824 0.

C 4.40504 -3.62136 1.06967

C 5.38875 -4.60749 1.07114

C 5.49381 -5.49381 0.

C 4.60749 -5.38875 -1.07114

C 3.62136 -4.40504 -1.06967

C -3.50824 -3.50824 0.

C -4.40504 -3.62136 1.06967

C -5.38875 -4.60749 1.07114

C -5.49381 -5.49381 0.

C -4.60749 -5.38875 -1.07114

C -3.62136 -4.40504 -1.06967

H -1.33092 5.12562 0.25983

H 1.33092 5.12562 0.25983

H 5.12562 -1.33092 -0.25983

H 5.12562 1.33092 -0.25983

H -5.12562 1.33092 -0.25983

H -5.12562 -1.33092 -0.25983

H -1.33092 -5.12562 0.25983

H 1.33092 -5.12562 0.25983

H 2.93697 4.32321 -1.90704

H 4.68458 6.07145 -1.91098

H 6.26099 6.26099 0.

H 6.07145 4.68458 1.91098

H 4.32321 2.93697 1.90704

H -6.26099 6.26099 0.

H -4.68458 6.07145 -1.91098

H -2.93697 4.32321 -1.90704

H -4.32321 2.93697 1.90704

H -6.07145 4.68458 1.91098

H 4.32321 -2.93697 1.90704

H 6.07145 -4.68458 1.91098

H 6.26099 -6.26099 0.

H 4.68458 -6.07145 -1.91098

H 2.93697 -4.32321 -1.90704

H -4.32321 -2.93697 1.90704

H -6.07145 -4.68458 1.91098

H -6.26099 -6.26099 0.

H -4.68458 -6.07145 -1.91098

H -2.93697 -4.32321 -1.90704

Zn 0. 0. 0.

NAtoms= 77 NQM= 77 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

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

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

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

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

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

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

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

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

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

Atom 11 12 13 14 15 16 17 18 19 20

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

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

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

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

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

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

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

Atom 21 22 23 24 25 26 27 28 29 30

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

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

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

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

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

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

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

Atom 31 32 33 34 35 36 37 38 39 40

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

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

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

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

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

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

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

Atom 41 42 43 44 45 46 47 48 49 50

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

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

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

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

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

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

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

Atom 51 52 53 54 55 56 57 58 59 60

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

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

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

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

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

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

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

Atom 61 62 63 64 65 66 67 68 69 70

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

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

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

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

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

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

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

Atom 71 72 73 74 75 76 77

IAtWgt= 1 1 1 1 1 1 64

AtmWgt= 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 63.9291454

NucSpn= 1 1 1 1 1 1 0

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 0.0000000

AtZNuc= 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 30.0000000

Leave Link 101 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 1.3

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

Stoichiometry C44H28N4Zn

Framework group D2D[O(Zn),2SGD(N2),X(C44H28)]

Deg. of freedom 29

Full point group D2D NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 -0.681484 4.269157 0.164086

2 6 0 -1.110541 2.890129 0.035503

3 7 0 0.000000 2.090529 -0.027459

4 6 0 1.110541 2.890129 0.035503

5 6 0 0.681484 4.269157 0.164086

6 6 0 2.452183 2.452183 0.000000

7 6 0 2.890129 1.110541 -0.035503

8 7 0 2.090529 0.000000 0.027459

9 6 0 2.890129 -1.110541 -0.035503

10 6 0 4.269157 -0.681484 -0.164086

11 6 0 4.269157 0.681484 -0.164086

12 6 0 -2.452183 2.452183 0.000000

13 6 0 -2.890129 1.110541 -0.035503

14 6 0 -4.269157 0.681484 -0.164086

15 6 0 -4.269157 -0.681484 -0.164086

16 6 0 -2.890129 -1.110541 -0.035503

17 7 0 -2.090529 0.000000 0.027459

18 6 0 -2.452183 -2.452183 0.000000

19 6 0 -1.110541 -2.890129 0.035503

20 6 0 -0.681484 -4.269157 0.164086

21 6 0 0.681484 -4.269157 0.164086

22 6 0 1.110541 -2.890129 0.035503

23 7 0 0.000000 -2.090529 -0.027459

24 6 0 2.452183 -2.452183 0.000000

25 6 0 3.508242 3.508242 0.000000

26 6 0 3.621357 4.405038 -1.069674

27 6 0 4.607485 5.388753 -1.071137

28 6 0 5.493806 5.493806 0.000000

29 6 0 5.388753 4.607485 1.071137

30 6 0 4.405038 3.621357 1.069674

31 6 0 -5.493806 5.493806 0.000000

32 6 0 -4.607485 5.388753 -1.071137

33 6 0 -3.621357 4.405038 -1.069674

34 6 0 -3.508242 3.508242 0.000000

35 6 0 -4.405038 3.621357 1.069674

36 6 0 -5.388753 4.607485 1.071137

37 6 0 3.508242 -3.508242 0.000000

38 6 0 4.405038 -3.621357 1.069674

39 6 0 5.388753 -4.607485 1.071137

40 6 0 5.493806 -5.493806 0.000000

41 6 0 4.607485 -5.388753 -1.071137

42 6 0 3.621357 -4.405038 -1.069674

43 6 0 -3.508242 -3.508242 0.000000

44 6 0 -4.405038 -3.621357 1.069674

45 6 0 -5.388753 -4.607485 1.071137

46 6 0 -5.493806 -5.493806 0.000000

47 6 0 -4.607485 -5.388753 -1.071137

48 6 0 -3.621357 -4.405038 -1.069674

49 1 0 -1.330917 5.125618 0.259828

50 1 0 1.330917 5.125618 0.259828

51 1 0 5.125618 -1.330917 -0.259828

52 1 0 5.125618 1.330917 -0.259828

53 1 0 -5.125618 1.330917 -0.259828

54 1 0 -5.125618 -1.330917 -0.259828

55 1 0 -1.330917 -5.125618 0.259828

56 1 0 1.330917 -5.125618 0.259828

57 1 0 2.936967 4.323214 -1.907040

58 1 0 4.684584 6.071446 -1.910980

59 1 0 6.260992 6.260992 0.000000

60 1 0 6.071446 4.684584 1.910980

61 1 0 4.323214 2.936967 1.907040

62 1 0 -6.260992 6.260992 0.000000

63 1 0 -4.684584 6.071446 -1.910980

64 1 0 -2.936967 4.323214 -1.907040

65 1 0 -4.323214 2.936967 1.907040

66 1 0 -6.071446 4.684584 1.910980

67 1 0 4.323214 -2.936967 1.907040

68 1 0 6.071446 -4.684584 1.910980

69 1 0 6.260992 -6.260992 0.000000

70 1 0 4.684584 -6.071446 -1.910980

71 1 0 2.936967 -4.323214 -1.907040

72 1 0 -4.323214 -2.936967 1.907040

73 1 0 -6.071446 -4.684584 1.910980

74 1 0 -6.260992 -6.260992 0.000000

75 1 0 -4.684584 -6.071446 -1.910980

76 1 0 -2.936967 -4.323214 -1.907040

77 30 0 0.000000 0.000000 0.000000

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

Rotational constants (GHZ): 0.0582110 0.0582110 0.0300828

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

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

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

Centers: 77

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: 49 50 51 52 53 54 55 56 57 58

Centers: 59 60 61 62 63 64 65 66 67 68

Centers: 69 70 71 72 73 74 75 76 1 2

Centers: 4 5 6 7 9 10 11 12 13 14

Centers: 15 16 18 19 20 21 22 24 25 26

Centers: 27 28 29 30 31 32 33 34 35 36

Centers: 37 38 39 40 41 42 43 44 45 46

Centers: 47 48 3 8 17 23

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 6

No pseudopotential on this center.

3 7

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 6

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 6

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 6

No pseudopotential on this center.

17 7

No pseudopotential on this center.

18 6

No pseudopotential on this center.

19 6

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 7

No pseudopotential on this center.

24 6

No pseudopotential on this center.

25 6

No pseudopotential on this center.

26 6

No pseudopotential on this center.

27 6

No pseudopotential on this center.

28 6

No pseudopotential on this center.

29 6

No pseudopotential on this center.

30 6

No pseudopotential on this center.

31 6

No pseudopotential on this center.

32 6

No pseudopotential on this center.

33 6

No pseudopotential on this center.

34 6

No pseudopotential on this center.

35 6

No pseudopotential on this center.

36 6

No pseudopotential on this center.

37 6

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38 6

No pseudopotential on this center.

39 6

No pseudopotential on this center.

40 6

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41 6

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42 6

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43 6

No pseudopotential on this center.

44 6

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45 6

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46 6

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47 6

No pseudopotential on this center.

48 6

No pseudopotential on this center.

49 1

No pseudopotential on this center.

50 1

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51 1

No pseudopotential on this center.

52 1

No pseudopotential on this center.

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67 1

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68 1

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69 1

No pseudopotential on this center.

70 1

No pseudopotential on this center.

71 1

No pseudopotential on this center.

72 1

No pseudopotential on this center.

73 1

No pseudopotential on this center.

74 1

No pseudopotential on this center.

75 1

No pseudopotential on this center.

76 1

No pseudopotential on this center.

77 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

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

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

There are 272 symmetry adapted cartesian basis functions of A1 symmetry.

There are 243 symmetry adapted cartesian basis functions of A2 symmetry.

There are 254 symmetry adapted cartesian basis functions of B1 symmetry.

There are 254 symmetry adapted cartesian basis functions of B2 symmetry.

There are 256 symmetry adapted basis functions of A1 symmetry.

There are 232 symmetry adapted basis functions of A2 symmetry.

There are 242 symmetry adapted basis functions of B1 symmetry.

There are 242 symmetry adapted basis functions of B2 symmetry.

972 basis functions, 1715 primitive gaussians, 1023 cartesian basis functions

166 alpha electrons 166 beta electrons

nuclear repulsion energy 5738.4943932451 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= 77 NActive= 77 NUniq= 13 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=T Big=F

Integral buffers will be 131072 words long.

Regular integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.2224135404 Hartrees.

Nuclear repulsion after empirical dispersion term = 5738.2719797046 Hartrees.

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

Polarizable Continuum Model (PCM)

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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= 77.

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

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

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

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

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

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

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

GePol: Number of generator spheres = 77

GePol: Total number of spheres = 77

GePol: Number of exposed spheres = 77 (100.00%)

GePol: Number of points = 5690

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.75D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 272

GePol: Fraction of low-weight points (<1% of avg) = 4.78%

GePol: Cavity surface area = 614.366 Ang\*\*2

GePol: Cavity volume = 630.258 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0025488972 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 5738.2694308075 Hartrees.

Leave Link 301 at Thu Sep 5 21:44:33 2019, MaxMem= 1342177280 cpu: 1.2

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

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

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

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 55278 NPrTT= 264852 LenC2= 36757 LenP2D= 95282.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 972 RedAO= T EigKep= 6.36D-05 NBF= 256 232 242 242

NBsUse= 972 1.00D-06 EigRej= -1.00D+00 NBFU= 256 232 242 242

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= 952 960 976 976 976 MxSgAt= 77 MxSgA2= 77.

Leave Link 302 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 19.9

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

Leave Link 308 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 2.9

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

DipDrv: MaxL=1.

Leave Link 303 at Thu Sep 5 21:44:35 2019, MaxMem= 1342177280 cpu: 1.9

(Enter /apps/gaussian/g09d01/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= -1979.25549734393

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Leave Link 401 at Thu Sep 5 21:44:38 2019, MaxMem= 1342177280 cpu: 36.9

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

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 3183261 IEndB= 3183261 NGot= 1342177280 MDV= 1340058212

LenX= 1340058212 LenY= 1339010660

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= 530000000 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= 97128300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 1.04D-14 for 1411.

Iteration 1 A\*A^-1 deviation from orthogonality is 5.32D-15 for 5415 1279.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.77D-15 for 448.

Iteration 1 A^-1\*A deviation from orthogonality is 4.87D-12 for 3423 3413.

E= -1977.86979971692

DIIS: error= 9.76D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1977.86979971692 IErMin= 1 ErrMin= 9.76D-02

ErrMax= 9.76D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.26D+00 BMatP= 1.26D+00

IDIUse=3 WtCom= 2.43D-02 WtEn= 9.76D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.106 Goal= None Shift= 0.000

GapD= 0.106 DampG=1.000 DampE=0.250 DampFc=0.2500 IDamp=-1.

Damping current iteration by 2.50D-01

RMSDP=1.86D-03 MaxDP=9.55D-02 OVMax= 1.55D-01

Cycle 2 Pass 1 IDiag 1:

RMSU= 4.59D-04 CP: 9.89D-01

E= -1978.23434090525 Delta-E= -0.364541188328 Rises=F Damp=T

DIIS: error= 4.17D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1978.23434090525 IErMin= 2 ErrMin= 4.17D-02

ErrMax= 4.17D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.72D-01 BMatP= 1.26D+00

IDIUse=3 WtCom= 5.83D-01 WtEn= 4.17D-01

Coeff-Com: -0.102D+01 0.202D+01

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

Coeff: -0.597D+00 0.160D+01

Gap= 0.102 Goal= None Shift= 0.000

RMSDP=7.18D-04 MaxDP=3.82D-02 DE=-3.65D-01 OVMax= 6.21D-02

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.10D-04 CP: 9.71D-01 2.26D+00

E= -1978.87163772524 Delta-E= -0.637296819993 Rises=F Damp=F

DIIS: error= 6.88D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1978.87163772524 IErMin= 3 ErrMin= 6.88D-03

ErrMax= 6.88D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.13D-02 BMatP= 3.72D-01

IDIUse=3 WtCom= 9.31D-01 WtEn= 6.88D-02

Coeff-Com: -0.858D-01 0.345D+00 0.741D+00

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

Coeff: -0.799D-01 0.321D+00 0.759D+00

Gap= 0.100 Goal= None Shift= 0.000

RMSDP=2.68D-04 MaxDP=1.66D-02 DE=-6.37D-01 OVMax= 3.62D-02

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.82D-04 CP: 9.77D-01 1.92D+00 7.16D-01

E= -1978.89712835253 Delta-E= -0.025490627289 Rises=F Damp=F

DIIS: error= 3.28D-03 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1978.89712835253 IErMin= 4 ErrMin= 3.28D-03

ErrMax= 3.28D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.50D-03 BMatP= 3.13D-02

IDIUse=3 WtCom= 9.67D-01 WtEn= 3.28D-02

Coeff-Com: 0.634D-01-0.345D-01 0.417D+00 0.554D+00

Coeff-En: 0.000D+00 0.000D+00 0.950D-01 0.905D+00

Coeff: 0.613D-01-0.334D-01 0.406D+00 0.566D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.13D-04 MaxDP=6.14D-03 DE=-2.55D-02 OVMax= 1.91D-02

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.90D-05 CP: 9.76D-01 1.96D+00 8.06D-01 5.28D-01

E= -1978.90379140222 Delta-E= -0.006663049687 Rises=F Damp=F

DIIS: error= 1.92D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1978.90379140222 IErMin= 5 ErrMin= 1.92D-03

ErrMax= 1.92D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.10D-03 BMatP= 7.50D-03

IDIUse=3 WtCom= 9.81D-01 WtEn= 1.92D-02

Coeff-Com: 0.422D-01-0.485D-01 0.173D+00 0.343D+00 0.491D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.680D-01 0.932D+00

Coeff: 0.414D-01-0.476D-01 0.169D+00 0.338D+00 0.500D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.24D-05 MaxDP=2.21D-03 DE=-6.66D-03 OVMax= 5.25D-03

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.69D-05 CP: 9.76D-01 1.97D+00 8.17D-01 5.92D-01 5.83D-01

E= -1978.90472522440 Delta-E= -0.000933822179 Rises=F Damp=F

DIIS: error= 6.56D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1978.90472522440 IErMin= 6 ErrMin= 6.56D-04

ErrMax= 6.56D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.82D-05 BMatP= 1.10D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.56D-03

Coeff-Com: 0.147D-01-0.196D-01 0.487D-01 0.118D+00 0.247D+00 0.591D+00

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

Coeff: 0.146D-01-0.195D-01 0.484D-01 0.118D+00 0.245D+00 0.593D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.46D-06 MaxDP=3.92D-04 DE=-9.34D-04 OVMax= 1.38D-03

Cycle 7 Pass 1 IDiag 1:

RMSU= 3.58D-06 CP: 9.76D-01 1.97D+00 8.19D-01 5.95D-01 6.09D-01

CP: 7.12D-01

E= -1978.90476135642 Delta-E= -0.000036132024 Rises=F Damp=F

DIIS: error= 7.60D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1978.90476135642 IErMin= 7 ErrMin= 7.60D-05

ErrMax= 7.60D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.73D-06 BMatP= 4.82D-05

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

Coeff-Com: 0.629D-02-0.867D-02 0.192D-01 0.502D-01 0.110D+00 0.307D+00

Coeff-Com: 0.515D+00

Coeff: 0.629D-02-0.867D-02 0.192D-01 0.502D-01 0.110D+00 0.307D+00

Coeff: 0.515D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.70D-06 MaxDP=7.88D-05 DE=-3.61D-05 OVMax= 4.51D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 1.19D-06 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.13D-01

CP: 7.19D-01 6.83D-01

E= -1978.90476361762 Delta-E= -0.000002261199 Rises=F Damp=F

DIIS: error= 2.12D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1978.90476361762 IErMin= 8 ErrMin= 2.12D-05

ErrMax= 2.12D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.42D-07 BMatP= 2.73D-06

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

Coeff-Com: 0.649D-03-0.956D-03 0.126D-02 0.492D-02 0.119D-01 0.498D-01

Coeff-Com: 0.246D+00 0.686D+00

Coeff: 0.649D-03-0.956D-03 0.126D-02 0.492D-02 0.119D-01 0.498D-01

Coeff: 0.246D+00 0.686D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=6.23D-07 MaxDP=2.40D-05 DE=-2.26D-06 OVMax= 1.20D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 4.02D-07 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

CP: 7.22D-01 7.38D-01 6.62D-01

E= -1978.90476381657 Delta-E= -0.000000198945 Rises=F Damp=F

DIIS: error= 1.32D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1978.90476381657 IErMin= 9 ErrMin= 1.32D-05

ErrMax= 1.32D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.21D-08 BMatP= 2.42D-07

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

Coeff-Com: 0.502D-04-0.108D-03-0.277D-03 0.863D-04 0.595D-03 0.106D-01

Coeff-Com: 0.105D+00 0.391D+00 0.493D+00

Coeff: 0.502D-04-0.108D-03-0.277D-03 0.863D-04 0.595D-03 0.106D-01

Coeff: 0.105D+00 0.391D+00 0.493D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.92D-07 MaxDP=9.22D-06 DE=-1.99D-07 OVMax= 3.07D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 8.99D-08 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

CP: 7.25D-01 7.48D-01 7.15D-01 6.86D-01

E= -1978.90476384796 Delta-E= -0.000000031398 Rises=F Damp=F

DIIS: error= 1.19D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1978.90476384796 IErMin=10 ErrMin= 1.19D-06

ErrMax= 1.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.75D-10 BMatP= 3.21D-08

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

Coeff-Com: -0.489D-04 0.598D-04-0.224D-03-0.474D-03-0.929D-03-0.611D-03

Coeff-Com: 0.158D-01 0.887D-01 0.160D+00 0.738D+00

Coeff: -0.489D-04 0.598D-04-0.224D-03-0.474D-03-0.929D-03-0.611D-03

Coeff: 0.158D-01 0.887D-01 0.160D+00 0.738D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=3.57D-08 MaxDP=1.68D-06 DE=-3.14D-08 OVMax= 6.26D-06

Cycle 11 Pass 1 IDiag 1:

RMSU= 2.73D-08 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

CP: 7.25D-01 7.50D-01 7.26D-01 7.02D-01 8.81D-01

E= -1978.90476384812 Delta-E= -0.000000000161 Rises=F Damp=F

DIIS: error= 9.44D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1978.90476384812 IErMin=11 ErrMin= 9.44D-07

ErrMax= 9.44D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.54D-10 BMatP= 6.75D-10

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

Coeff-Com: -0.301D-04 0.401D-04-0.965D-04-0.269D-03-0.542D-03-0.119D-02

Coeff-Com: -0.338D-03 0.174D-01 0.479D-01 0.432D+00 0.505D+00

Coeff: -0.301D-04 0.401D-04-0.965D-04-0.269D-03-0.542D-03-0.119D-02

Coeff: -0.338D-03 0.174D-01 0.479D-01 0.432D+00 0.505D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=1.48D-08 MaxDP=8.48D-07 DE=-1.61D-10 OVMax= 3.20D-06

Cycle 12 Pass 1 IDiag 1:

RMSU= 7.03D-09 CP: 9.76D-01 1.97D+00 8.19D-01 5.97D-01 6.15D-01

CP: 7.25D-01 7.50D-01 7.29D-01 7.04D-01 9.29D-01

CP: 6.54D-01

E= -1978.90476384822 Delta-E= -0.000000000100 Rises=F Damp=F

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

NSaved=12 IEnMin=12 EnMin= -1978.90476384822 IErMin=12 ErrMin= 1.51D-07

ErrMax= 1.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.86D-12 BMatP= 2.54D-10

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

Coeff-Com: -0.467D-05 0.644D-05-0.108D-04-0.471D-04-0.838D-04-0.299D-03

Coeff-Com: -0.128D-02-0.148D-02 0.230D-02 0.616D-01 0.135D+00 0.805D+00

Coeff: -0.467D-05 0.644D-05-0.108D-04-0.471D-04-0.838D-04-0.299D-03

Coeff: -0.128D-02-0.148D-02 0.230D-02 0.616D-01 0.135D+00 0.805D+00

Gap= 0.099 Goal= None Shift= 0.000

RMSDP=2.71D-09 MaxDP=1.31D-07 DE=-1.00D-10 OVMax= 4.01D-07

Error on total polarization charges = 0.08494

SCF Done: E(RB3LYP) = -1978.90476385 A.U. after 12 cycles

NFock= 12 Conv=0.27D-08 -V/T= 1.9793

KE= 2.020706235307D+03 PE=-1.615865212455D+04 EE= 6.420771694589D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.60

(included in total energy above)

Leave Link 502 at Thu Sep 5 21:47:21 2019, MaxMem= 1342177280 cpu: 1883.0

(Enter /apps/gaussian/g09d01/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 4.98D-05

Largest core mixing into a valence orbital is 2.06D-05

Range of M.O.s used for correlation: 49 972

NBasis= 972 NAE= 166 NBE= 166 NFC= 48 NFV= 0

NROrb= 924 NOA= 118 NOB= 118 NVA= 806 NVB= 806

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.98725075D-01

Leave Link 801 at Thu Sep 5 21:47:22 2019, MaxMem= 1342177280 cpu: 3.9

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

RHF ground state

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

Would need an additional 138418000000 words for in-memory AO integral storage.

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

Inv3: Mode=1 IEnd= 97128300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 9.33D-15 for 423.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.84D-15 for 5688 2045.

Iteration 1 A^-1\*A deviation from unit magnitude is 8.88D-15 for 5689.

Iteration 1 A^-1\*A deviation from orthogonality is 2.30D-15 for 5114 1632.

Making orbital integer symmetry assigments:

Orbital symmetries:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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: 190216

Iteration 1 Dimension 40 NMult 0 NNew 40

CISAX will form 40 AO SS matrices at one time.

NMat= 40 NSing= 40 JSym2X=-1.

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

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

New state 1 was old state 2

New state 2 was old state 1

New state 3 was old state 4

New state 4 was old state 3

New state 5 was old state 10

New state 6 was old state 19

New state 7 was old state 18

New state 8 was old state 9

New state 9 was old state 7

New state 10 was old state 6

Excitation Energies [eV] at current iteration:

Root 1 : 2.428701294553804

Root 2 : 2.428701294561318

Root 3 : 3.516587131283769

Root 4 : 3.516587131292371

Root 5 : 3.737574948387520

Root 6 : 3.751474798011214

Root 7 : 3.751474798016408

Root 8 : 3.789777221301642

Root 9 : 3.860011255053419

Root 10 : 3.860011255054868

Root 11 : 3.879928141245375

Root 12 : 3.928861122070199

Root 13 : 3.935043775686835

Root 14 : 3.938391550040616

Root 15 : 3.944965103579341

Root 16 : 3.944965103585384

Root 17 : 3.998792379426353

Root 18 : 4.079214263132060

Root 19 : 4.118984688881808

Root 20 : 4.121102407888769

Root 21 : 4.129997545101186

Root 22 : 4.129997545108232

Root 23 : 4.144646121011398

Root 24 : 4.144646121012867

Root 25 : 4.157208570676358

Root 26 : 4.190411636358658

Root 27 : 4.195110218156840

Root 28 : 4.195110218160975

Root 29 : 4.248641871883007

Root 30 : 4.344998820039009

Root 31 : 4.344998820046047

Root 32 : 4.407450143252086

Root 33 : 4.409214275449306

Root 34 : 4.409214275451562

Root 35 : 4.415812279712141

Root 36 : 4.430910757956899

Root 37 : 4.570937252676748

Root 38 : 4.627142328889381

Root 39 : 4.627142328890429

Root 40 : 4.687171051634622

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 0.048276419240189

Root 2 not converged, maximum delta is 0.048276419239130

New state 3 was old state 4

Root 3 not converged, maximum delta is 0.105237263631832

New state 4 was old state 3

Root 4 not converged, maximum delta is 0.105237263629962

Root 5 not converged, maximum delta is 0.132956633013194

New state 6 was old state 9

Root 6 not converged, maximum delta is 0.120857581823096

New state 7 was old state 10

Root 7 not converged, maximum delta is 0.120857581819533

Root 8 not converged, maximum delta is 0.183429470331180

New state 9 was old state 6

Root 9 not converged, maximum delta is 0.047187505572209

New state 10 was old state 7

Root 10 not converged, maximum delta is 0.047187505575253

Excitation Energies [eV] at current iteration:

Root 1 : 2.219662329494617 Change is -0.209038965059187

Root 2 : 2.219662329504469 Change is -0.209038965056849

Root 3 : 3.057934722647806 Change is -0.458652408644565

Root 4 : 3.057934722648881 Change is -0.458652408634888

Root 5 : 3.589271617406991 Change is -0.148303330980529

Root 6 : 3.649480729468749 Change is -0.210530525584670

Root 7 : 3.649480729473795 Change is -0.210530525581073

Root 8 : 3.656750818764339 Change is -0.133026402537303

Root 9 : 3.716296741982316 Change is -0.035178056028898

Root 10 : 3.716296741986607 Change is -0.035178056029801

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 0.004224161675550

Root 2 not converged, maximum delta is 0.004224161675043

Root 3 not converged, maximum delta is 0.012616494209895

Root 4 not converged, maximum delta is 0.012616494209733

Root 5 not converged, maximum delta is 0.019469229625695

New state 6 was old state 8

Root 6 not converged, maximum delta is 0.131404927576437

New state 7 was old state 6

Root 7 not converged, maximum delta is 0.015169229143350

New state 8 was old state 7

Root 8 not converged, maximum delta is 0.015169229141824

Root 9 not converged, maximum delta is 0.009160397667692

Root 10 not converged, maximum delta is 0.009160397667312

Excitation Energies [eV] at current iteration:

Root 1 : 2.209051626711254 Change is -0.010610702783364

Root 2 : 2.209051626721525 Change is -0.010610702782944

Root 3 : 3.026251031978266 Change is -0.031683690669540

Root 4 : 3.026251031979597 Change is -0.031683690669284

Root 5 : 3.579007642490882 Change is -0.010263974916109

Root 6 : 3.636322320972348 Change is -0.020428497791991

Root 7 : 3.642866428769356 Change is -0.006614300699393

Root 8 : 3.642866428774614 Change is -0.006614300699181

Root 9 : 3.714492876456073 Change is -0.001803865526242

Root 10 : 3.714492876460456 Change is -0.001803865526152

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 0.002979685217567

Root 2 not converged, maximum delta is 0.002979685217440

Root 3 not converged, maximum delta is 0.005551206197589

Root 4 not converged, maximum delta is 0.005551206196308

Root 5 not converged, maximum delta is 0.006108026759717

Root 6 not converged, maximum delta is 0.137130930300203

Root 7 not converged, maximum delta is 0.004614856418706

Root 8 not converged, maximum delta is 0.004614856416389

Root 9 not converged, maximum delta is 0.001985301489102

Root 10 not converged, maximum delta is 0.001985301489655

Excitation Energies [eV] at current iteration:

Root 1 : 2.207557240907411 Change is -0.001494385803843

Root 2 : 2.207557240917094 Change is -0.001494385804431

Root 3 : 3.022533831082758 Change is -0.003717200895508

Root 4 : 3.022533831083873 Change is -0.003717200895724

Root 5 : 3.577196714157072 Change is -0.001810928333810

Root 6 : 3.622657187266614 Change is -0.013665133705735

Root 7 : 3.641564982906088 Change is -0.001301445863268

Root 8 : 3.641564982911596 Change is -0.001301445863018

Root 9 : 3.714225483995815 Change is -0.000267392460259

Root 10 : 3.714225484000153 Change is -0.000267392460303

Iteration 5 Dimension 120 NMult 100 NNew 20

CISAX will form 20 AO SS matrices at one time.

NMat= 20 NSing= 20 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 not converged, maximum delta is 0.001138719065031

Root 4 not converged, maximum delta is 0.001138719061672

Root 5 not converged, maximum delta is 0.001888205760320

Root 6 not converged, maximum delta is 0.032875977975611

Root 7 has converged.

Root 8 has converged.

Root 9 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 2.207461215948761 Change is -0.000096024958650

Root 2 : 2.207461215958519 Change is -0.000096024958575

Root 3 : 3.022193158796154 Change is -0.000340672286604

Root 4 : 3.022193158797704 Change is -0.000340672286168

Root 5 : 3.576961078757767 Change is -0.000235635399306

Root 6 : 3.620299360922235 Change is -0.002357826344378

Root 7 : 3.641458425233346 Change is -0.000106557672742

Root 8 : 3.641458425239081 Change is -0.000106557672515

Root 9 : 3.714194035352776 Change is -0.000031448643039

Root 10 : 3.714194035357092 Change is -0.000031448643061

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 not converged, maximum delta is 0.069273011040973

Root 4 not converged, maximum delta is 0.069273011041752

Root 5 has converged.

Root 6 not converged, maximum delta is 0.013795277892522

Root 7 not converged, maximum delta is 0.001176016707628

Root 8 not converged, maximum delta is 0.001176016707622

Root 9 not converged, maximum delta is 0.002309641306672

Root 10 not converged, maximum delta is 0.002309641306663

Excitation Energies [eV] at current iteration:

Root 1 : 2.207459660537243 Change is -0.000001555411518

Root 2 : 2.207459660546926 Change is -0.000001555411593

Root 3 : 3.022172199503860 Change is -0.000020959292294

Root 4 : 3.022172199505383 Change is -0.000020959292322

Root 5 : 3.576933084223689 Change is -0.000027994534078

Root 6 : 3.619781110777733 Change is -0.000518250144502

Root 7 : 3.641456779454625 Change is -0.000001645778721

Root 8 : 3.641456779460427 Change is -0.000001645778654

Root 9 : 3.714193574807802 Change is -0.000000460544974

Root 10 : 3.714193574812140 Change is -0.000000460544952

Iteration 7 Dimension 142 NMult 128 NNew 14

CISAX will form 14 AO SS matrices at one time.

NMat= 14 NSing= 14 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 not converged, maximum delta is 0.069273010717385

Root 4 not converged, maximum delta is 0.069273010718170

Root 5 has converged.

Root 6 not converged, maximum delta is 0.001907212971949

Root 7 not converged, maximum delta is 0.001176016707949

Root 8 not converged, maximum delta is 0.001176016707944

Root 9 not converged, maximum delta is 0.002309641305933

Root 10 not converged, maximum delta is 0.002309641305904

Excitation Energies [eV] at current iteration:

Root 1 : 2.207458717972577 Change is -0.000000942564666

Root 2 : 2.207458717982148 Change is -0.000000942564778

Root 3 : 3.022170994057352 Change is -0.000001205446508

Root 4 : 3.022170994058930 Change is -0.000001205446453

Root 5 : 3.576933084223759 Change is 0.000000000000069

Root 6 : 3.619703435680521 Change is -0.000077675097212

Root 7 : 3.641447168529113 Change is -0.000009610925513

Root 8 : 3.641447168534869 Change is -0.000009610925558

Root 9 : 3.714190896727137 Change is -0.000002678080665

Root 10 : 3.714190896731497 Change is -0.000002678080643

Iteration 8 Dimension 156 NMult 142 NNew 14

CISAX will form 14 AO SS matrices at one time.

NMat= 14 NSing= 14 JSym2X=-1.

Root 1 has converged.

Root 2 has converged.

Root 3 has converged.

Root 4 has converged.

Root 5 has converged.

Root 6 has converged.

Root 7 has converged.

Root 8 has converged.

Root 9 has converged.

Root 10 has converged.

Excitation Energies [eV] at current iteration:

Root 1 : 2.207458321695631 Change is -0.000000396276946

Root 2 : 2.207458321705350 Change is -0.000000396276798

Root 3 : 3.022170891506403 Change is -0.000000102550950

Root 4 : 3.022170891508007 Change is -0.000000102550922

Root 5 : 3.576933084223667 Change is -0.000000000000092

Root 6 : 3.619695293052603 Change is -0.000008142627919

Root 7 : 3.641446389572518 Change is -0.000000778956595

Root 8 : 3.641446389578229 Change is -0.000000778956640

Root 9 : 3.714190651491251 Change is -0.000000245235886

Root 10 : 3.714190651495456 Change is -0.000000245236041

Convergence achieved on expansion vectors.

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

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

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

1PDM for each excited state written to RWF 633

Ground to excited state transition densities written to RWF 633

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

state X Y Z Dip. S. Osc.

1 -1.0775 0.0000 0.0000 1.1609 0.0628

2 0.0000 -1.0775 0.0000 1.1609 0.0628

3 4.7181 0.0000 0.0000 22.2607 1.6482

4 0.0000 -4.7181 0.0000 22.2607 1.6482

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 -0.7214 0.0000 0.0000 0.5205 0.0464

8 0.0000 0.7214 0.0000 0.5205 0.0464

9 0.5065 0.0000 0.0000 0.2566 0.0233

10 0.0000 0.5065 0.0000 0.2566 0.0233

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

state X Y Z Dip. S. Osc.

1 0.0834 0.0000 0.0000 0.0070 0.0572

2 0.0000 0.0834 0.0000 0.0070 0.0572

3 -0.5158 0.0000 0.0000 0.2660 1.5969

4 0.0000 0.5158 0.0000 0.2660 1.5969

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 0.0973 0.0000 0.0000 0.0095 0.0472

8 0.0000 -0.0973 0.0000 0.0095 0.0472

9 -0.0677 0.0000 0.0000 0.0046 0.0224

10 0.0000 -0.0677 0.0000 0.0046 0.0224

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

state X Y Z

1 0.0000 -0.0326 0.0000

2 -0.0326 0.0000 0.0000

3 0.0000 -0.0024 0.0000

4 0.0024 0.0000 0.0000

5 0.0000 0.0000 -2.2513

6 0.0000 0.0000 0.0000

7 0.0000 0.1101 0.0000

8 -0.1101 0.0000 0.0000

9 0.0000 -0.3690 0.0000

10 -0.3690 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 0.0459 0.0000

2 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0459

3 0.0000 0.0000 0.0000 0.0000 0.0255 0.0000

4 0.0000 0.0000 0.0000 0.0000 0.0000 0.0255

5 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 -0.6486 0.0000 0.0000

7 0.0000 0.0000 0.0000 0.0000 0.0166 0.0000

8 0.0000 0.0000 0.0000 0.0000 0.0000 0.0166

9 0.0000 0.0000 0.0000 0.0000 -0.0569 0.0000

10 0.0000 0.0000 0.0000 0.0000 0.0000 0.0569

<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 -0.0899 0.0000 0.0000 0.0899 0.0599

2 0.0000 -0.0899 0.0000 0.0899 0.0599

3 -2.4336 0.0000 0.0000 2.4336 1.6224

4 0.0000 -2.4336 0.0000 2.4336 1.6224

5 0.0000 0.0000 0.0000 0.0000 0.0000

6 0.0000 0.0000 0.0000 0.0000 0.0000

7 -0.0702 0.0000 0.0000 0.0702 0.0468

8 0.0000 -0.0702 0.0000 0.0702 0.0468

9 -0.0343 0.0000 0.0000 0.0343 0.0229

10 0.0000 -0.0343 0.0000 0.0343 0.0229

Excitation energies and oscillator strengths:

Excited State 1: Singlet-E 2.2075 eV 561.66 nm f=0.0628 <S\*\*2>=0.000

52 ->237 0.00106

57 ->228 0.00122

58 ->226 -0.00111

58 ->258 0.00114

58 ->273 -0.00108

58 ->280 0.00108

59 ->225 -0.00142

59 ->232 0.00163

59 ->268 -0.00136

60 ->229 0.00144

60 ->237 0.00142

72 ->224 0.00110

72 ->228 -0.00156

73 ->229 0.00162

73 ->237 0.00130

73 ->271 -0.00119

74 ->226 0.00132

74 ->231 0.00125

74 ->247 -0.00110

74 ->258 -0.00153

74 ->273 0.00150

74 ->296 -0.00100

75 ->225 -0.00121

75 ->236 -0.00170

75 ->317 -0.00147

76 ->228 0.00106

76 ->238 0.00105

84 ->238 0.00109

84 ->257 -0.00106

84 ->262 0.00128

85 ->246 -0.00102

85 ->322 -0.00122

86 ->322 0.00132

86 ->325 -0.00112

88 ->226 0.00111

88 ->285 0.00114

90 ->228 -0.00176

94 ->238 0.00107

95 ->226 -0.00115

95 ->341 0.00148

100 ->186 0.00116

100 ->194 0.00122

100 ->197 0.00104

101 ->181 -0.00103

101 ->228 0.00161

103 ->226 0.00228

103 ->341 -0.00197

103 ->347 0.00131

104 ->180 0.00103

104 ->225 0.00116

104 ->232 -0.00108

104 ->268 0.00114

104 ->317 -0.00103

105 ->217 0.00129

106 ->167 -0.00203

106 ->249 -0.00164

106 ->349 -0.00112

107 ->168 -0.00241

107 ->204 0.00205

107 ->220 0.00108

108 ->169 -0.00248

108 ->200 -0.00148

109 ->205 0.00106

110 ->169 -0.00121

110 ->226 0.00106

110 ->231 0.00100

110 ->341 -0.00102

111 ->170 -0.00118

111 ->198 -0.00101

111 ->232 -0.00106

112 ->228 -0.00151

113 ->167 0.00215

113 ->172 0.00109

113 ->234 -0.00150

113 ->249 -0.00147

113 ->257 0.00184

113 ->315 0.00106

113 ->320 0.00129

113 ->324 0.00150

113 ->349 -0.00194

113 ->368 0.00123

114 ->223 -0.00189

115 ->168 -0.00447

115 ->204 0.00194

115 ->220 0.00143

116 ->169 -0.00103

116 ->193 -0.00114

116 ->231 -0.00122

117 ->190 -0.00106

118 ->191 -0.00119

119 ->170 0.00104

119 ->222 -0.00109

119 ->225 -0.00108

119 ->260 -0.00113

120 ->169 0.00148

120 ->231 -0.00212

120 ->233 0.00102

121 ->229 0.00143

121 ->237 0.00152

122 ->168 -0.00551

122 ->192 -0.00107

122 ->204 0.00245

122 ->220 0.00113

123 ->224 0.00123

123 ->228 -0.00161

123 ->249 -0.00123

123 ->257 0.00178

123 ->278 0.00106

123 ->305 0.00117

123 ->315 -0.00106

124 ->205 0.00156

124 ->210 0.00101

124 ->227 0.00127

125 ->169 -0.00659

125 ->175 -0.00161

125 ->193 0.00128

125 ->200 -0.00333

125 ->221 -0.00148

125 ->326 -0.00102

126 ->180 0.00111

126 ->186 0.00105

126 ->230 0.00102

126 ->253 0.00106

126 ->308 0.00123

126 ->317 -0.00133

126 ->406 -0.00109

127 ->240 0.00143

127 ->258 0.00140

127 ->341 -0.00109

128 ->168 -0.00529

128 ->176 -0.00117

128 ->204 0.00142

128 ->220 0.00104

129 ->228 -0.00151

130 ->322 -0.00107

130 ->325 0.00159

130 ->350 -0.00103

131 ->167 -0.00168

131 ->172 -0.00124

132 ->276 -0.00133

132 ->285 -0.00160

132 ->293 -0.00100

132 ->341 -0.00112

133 ->180 0.00113

133 ->230 0.00101

133 ->259 0.00126

133 ->317 -0.00125

134 ->168 -0.00159

134 ->171 0.00115

134 ->271 0.00100

135 ->229 -0.00118

136 ->197 0.00106

136 ->236 -0.00114

137 ->175 -0.00113

137 ->341 -0.00116

138 ->167 -0.00335

138 ->219 -0.00119

138 ->257 0.00103

138 ->324 0.00102

139 ->201 0.00178

139 ->223 0.00168

139 ->237 0.00100

139 ->246 0.00114

140 ->167 0.00581

140 ->203 0.00188

141 ->185 0.00102

141 ->199 -0.00102

141 ->231 -0.00195

141 ->233 0.00113

142 ->198 0.00133

142 ->222 -0.00119

142 ->253 -0.00105

143 ->204 -0.00127

144 ->231 -0.00156

144 ->244 0.00104

145 ->170 0.00134

145 ->186 -0.00108

145 ->198 0.00127

145 ->210 0.00127

145 ->253 -0.00101

146 ->172 0.00147

146 ->181 -0.00126

146 ->202 0.00112

146 ->208 -0.00115

146 ->224 0.00109

146 ->228 -0.00146

146 ->234 0.00133

146 ->238 0.00174

146 ->249 -0.00148

146 ->257 0.00205

146 ->270 0.00109

147 ->167 -0.01998

147 ->172 0.00203

147 ->177 0.00141

147 ->203 -0.00207

147 ->211 -0.00176

147 ->219 -0.00213

147 ->266 -0.00102

148 ->169 0.00138

148 ->226 -0.00164

148 ->240 0.00113

149 ->179 -0.00228

149 ->180 -0.00281

149 ->186 -0.00277

149 ->194 -0.00201

149 ->213 -0.00116

149 ->225 -0.00230

149 ->236 -0.00210

149 ->250 0.00104

149 ->253 -0.00119

149 ->277 -0.00143

149 ->309 -0.00109

149 ->317 -0.00103

149 ->366 0.00130

149 ->378 -0.00121

150 ->169 0.00265

150 ->189 0.00126

151 ->174 0.00402

151 ->178 0.00320

151 ->179 -0.01218

151 ->180 0.00394

151 ->190 0.00187

151 ->197 -0.00247

151 ->205 -0.00610

151 ->216 -0.00251

151 ->227 -0.00169

151 ->274 -0.00146

151 ->370 -0.00121

152 ->168 0.00279

152 ->171 -0.00339

152 ->176 -0.00170

152 ->183 0.00552

152 ->201 0.00132

152 ->204 -0.00369

152 ->207 0.00115

152 ->212 -0.00177

152 ->220 -0.00180

153 ->168 -0.00158

153 ->171 -0.00224

153 ->176 -0.00131

153 ->183 -0.00371

153 ->204 0.00178

153 ->220 0.00107

153 ->223 0.00111

153 ->246 -0.00107

153 ->248 -0.00135

153 ->271 -0.00163

154 ->168 0.01082

154 ->171 0.00143

154 ->176 -0.00193

154 ->183 -0.00135

154 ->204 0.00114

155 ->167 -0.00727

155 ->172 0.00211

155 ->177 -0.00186

155 ->184 0.00153

156 ->169 0.00156

156 ->173 0.00245

156 ->175 0.00195

157 ->170 -0.00203

157 ->174 -0.00306

157 ->179 0.00182

158 ->168 0.01096

158 ->171 0.00191

158 ->176 0.00144

158 ->183 0.00258

158 ->220 -0.00114

158 ->223 0.00157

158 ->229 0.00183

158 ->235 -0.00123

158 ->237 -0.00104

158 ->263 -0.00143

158 ->271 -0.00105

159 ->167 -0.00503

159 ->172 0.00595

159 ->177 0.00228

159 ->208 -0.00128

160 ->170 0.00311

160 ->174 0.00178

160 ->179 -0.01000

160 ->180 0.00293

160 ->190 0.00109

160 ->205 -0.00289

160 ->216 -0.00211

160 ->227 -0.00137

160 ->236 -0.00156

160 ->283 0.00100

161 ->169 -0.00344

161 ->173 -0.00141

161 ->175 0.00537

161 ->209 -0.00104

162 ->170 0.00486

162 ->174 0.00125

162 ->178 0.00310

162 ->210 0.00123

162 ->227 0.00182

163 ->169 -0.01640

163 ->173 -0.00108

163 ->189 -0.00344

164 ->168 -0.03390

164 ->171 -0.00277

164 ->176 -0.00298

164 ->183 0.00328

164 ->201 0.00119

164 ->204 -0.00381

164 ->212 -0.00121

164 ->220 -0.00221

165 ->167 0.39512

165 ->172 -0.00284

165 ->177 -0.00693

165 ->184 -0.01146

165 ->203 0.00319

165 ->208 -0.00115

165 ->211 0.00166

165 ->219 0.00230

165 ->249 -0.00106

166 ->168 0.58445

166 ->171 0.00149

166 ->176 0.00197

166 ->183 -0.00801

166 ->201 -0.00175

166 ->204 0.00739

166 ->212 0.00305

166 ->217 0.00176

166 ->220 0.00549

166 ->265 0.00194

166 ->335 -0.00110

166 ->345 -0.00111

57 <-228 0.00107

58 <-258 0.00100

59 <-225 -0.00121

59 <-232 0.00141

59 <-268 -0.00118

60 <-229 0.00122

60 <-237 0.00122

72 <-228 -0.00132

73 <-229 0.00135

73 <-237 0.00111

73 <-271 -0.00103

74 <-226 0.00107

74 <-231 0.00105

74 <-258 -0.00130

74 <-273 0.00128

75 <-236 -0.00142

75 <-317 -0.00125

84 <-262 0.00108

85 <-322 -0.00107

86 <-322 0.00114

90 <-228 -0.00141

95 <-341 0.00126

101 <-228 0.00126

103 <-226 0.00175

103 <-341 -0.00167

103 <-347 0.00112

106 <-167 -0.00129

106 <-249 -0.00128

107 <-168 -0.00198

107 <-204 0.00165

108 <-169 -0.00192

108 <-200 -0.00119

112 <-228 -0.00118

113 <-167 0.00132

113 <-234 -0.00116

113 <-249 -0.00121

113 <-257 0.00146

113 <-320 0.00106

113 <-324 0.00123

113 <-349 -0.00164

113 <-368 0.00105

114 <-223 -0.00140

115 <-168 -0.00248

115 <-204 0.00167

115 <-220 0.00119

120 <-231 -0.00161

121 <-229 0.00108

121 <-237 0.00118

122 <-168 -0.00256

122 <-204 0.00204

123 <-228 -0.00123

123 <-257 0.00140

124 <-205 0.00151

124 <-227 0.00134

125 <-169 -0.00393

125 <-200 -0.00247

125 <-221 -0.00117

126 <-308 0.00100

126 <-317 -0.00110

127 <-240 0.00111

127 <-258 0.00108

128 <-168 -0.00198

129 <-228 -0.00116

130 <-325 0.00132

132 <-276 -0.00107

132 <-285 -0.00130

133 <-317 -0.00102

138 <-167 -0.00180

139 <-201 0.00117

139 <-223 0.00118

140 <-167 0.00318

140 <-203 0.00168

141 <-231 -0.00140

144 <-231 -0.00113

146 <-228 -0.00111

146 <-238 0.00128

146 <-249 -0.00113

146 <-257 0.00157

147 <-167 -0.01052

147 <-184 -0.00175

147 <-203 -0.00274

147 <-211 -0.00160

147 <-219 -0.00197

148 <-226 -0.00116

149 <-180 -0.00193

149 <-186 -0.00175

149 <-194 -0.00133

149 <-225 -0.00163

149 <-236 -0.00155

149 <-277 -0.00115

149 <-366 0.00107

150 <-169 -0.00524

150 <-189 0.00113

150 <-200 -0.00103

151 <-174 0.00117

151 <-178 0.00218

151 <-179 -0.00355

151 <-180 0.00120

151 <-190 0.00132

151 <-197 -0.00180

151 <-205 -0.00452

151 <-216 -0.00186

151 <-227 -0.00143

151 <-274 -0.00123

151 <-370 -0.00107

152 <-171 -0.00148

152 <-183 0.00336

152 <-204 -0.00208

152 <-212 -0.00103

153 <-168 0.00300

153 <-183 -0.00244

153 <-271 -0.00127

154 <-168 0.00226

155 <-167 -0.00198

157 <-174 -0.00125

157 <-179 0.00150

158 <-168 -0.00233

158 <-183 0.00226

158 <-229 0.00120

158 <-263 -0.00104

159 <-167 -0.00305

159 <-172 0.00188

159 <-177 0.00110

160 <-170 0.00109

160 <-179 -0.00418

160 <-180 0.00120

160 <-205 -0.00193

160 <-216 -0.00139

160 <-227 -0.00113

160 <-236 -0.00114

161 <-169 0.00128

161 <-175 0.00248

162 <-170 0.00148

162 <-178 0.00206

162 <-179 0.00337

162 <-180 -0.00100

162 <-227 0.00116

163 <-189 -0.00200

164 <-168 -0.00699

164 <-171 -0.00108

164 <-176 -0.00106

164 <-183 0.00188

164 <-204 -0.00262

164 <-220 -0.00160

165 <-167 0.02993

165 <-177 -0.00206

165 <-184 -0.00601

165 <-203 0.00238

165 <-211 0.00103

165 <-219 0.00190

166 <-168 -0.01163

166 <-183 -0.00245

166 <-201 -0.00106

166 <-204 0.00415

166 <-212 0.00220

166 <-220 0.00316

166 <-265 0.00163

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

Total Energy, E(TD-HF/TD-KS) = -1978.82364124

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

Excited State 2: Singlet-E 2.2075 eV 561.66 nm f=0.0628 <S\*\*2>=0.000

52 ->238 -0.00106

57 ->229 0.00122

58 ->225 -0.00142

58 ->232 0.00163

58 ->268 -0.00136

59 ->226 -0.00111

59 ->258 0.00114

59 ->273 -0.00108

59 ->280 0.00108

60 ->228 0.00144

60 ->238 0.00142

72 ->223 -0.00110

72 ->229 0.00156

73 ->228 0.00162

73 ->238 0.00130

73 ->272 0.00119

74 ->225 0.00121

74 ->236 -0.00170

74 ->317 -0.00147

75 ->226 -0.00132

75 ->231 -0.00125

75 ->247 0.00110

75 ->258 0.00153

75 ->273 -0.00150

75 ->296 0.00100

76 ->229 0.00106

76 ->237 0.00105

84 ->237 0.00109

84 ->256 -0.00106

84 ->263 0.00128

85 ->245 0.00102

85 ->323 0.00122

86 ->323 -0.00132

86 ->324 0.00112

89 ->226 0.00111

89 ->285 -0.00114

90 ->229 -0.00176

94 ->237 0.00107

96 ->226 -0.00115

96 ->341 -0.00148

99 ->186 0.00116

99 ->194 0.00122

99 ->197 -0.00104

101 ->182 -0.00103

101 ->229 0.00161

103 ->180 0.00103

103 ->225 0.00116

103 ->232 -0.00108

103 ->268 0.00114

103 ->317 0.00103

104 ->226 0.00228

104 ->341 0.00197

104 ->347 -0.00131

105 ->218 0.00129

106 ->168 -0.00203

106 ->248 0.00164

106 ->350 0.00112

107 ->167 -0.00241

107 ->203 -0.00205

107 ->219 -0.00108

108 ->205 0.00106

109 ->169 -0.00248

109 ->200 -0.00148

110 ->170 0.00118

110 ->198 -0.00101

110 ->232 -0.00106

111 ->169 0.00121

111 ->226 0.00106

111 ->231 0.00100

111 ->341 0.00102

112 ->229 -0.00151

113 ->168 0.00215

113 ->171 -0.00109

113 ->235 0.00150

113 ->248 0.00147

113 ->256 -0.00184

113 ->316 -0.00106

113 ->321 -0.00129

113 ->325 -0.00150

113 ->350 0.00194

113 ->369 -0.00123

114 ->224 -0.00189

115 ->167 -0.00447

115 ->203 -0.00194

115 ->219 -0.00143

116 ->190 -0.00106

117 ->169 -0.00103

117 ->193 -0.00114

117 ->231 0.00122

118 ->192 0.00119

119 ->169 -0.00148

119 ->231 -0.00212

119 ->233 0.00102

120 ->170 -0.00104

120 ->222 -0.00109

120 ->225 -0.00108

120 ->260 -0.00113

121 ->228 0.00143

121 ->238 0.00152

122 ->167 -0.00551

122 ->191 0.00107

122 ->203 -0.00245

122 ->219 -0.00113

123 ->223 0.00123

123 ->229 -0.00161

123 ->248 -0.00123

123 ->256 0.00178

123 ->279 0.00106

123 ->304 -0.00117

123 ->316 -0.00106

124 ->169 -0.00659

124 ->175 -0.00161

124 ->193 0.00128

124 ->200 -0.00333

124 ->221 -0.00148

124 ->326 -0.00102

125 ->205 0.00156

125 ->210 0.00101

125 ->227 0.00127

126 ->240 -0.00143

126 ->258 0.00140

126 ->341 0.00109

127 ->180 0.00111

127 ->186 0.00105

127 ->230 -0.00102

127 ->253 0.00106

127 ->308 0.00123

127 ->317 0.00133

127 ->406 0.00109

128 ->167 0.00529

128 ->177 -0.00117

128 ->203 0.00142

128 ->219 0.00104

129 ->229 -0.00151

130 ->323 0.00107

130 ->324 -0.00159

130 ->349 0.00103

131 ->168 -0.00168

131 ->171 0.00124

132 ->180 0.00113

132 ->230 -0.00101

132 ->259 -0.00126

132 ->317 0.00125

133 ->276 0.00133

133 ->285 0.00160

133 ->293 0.00100

133 ->341 0.00112

134 ->167 -0.00159

134 ->172 -0.00115

134 ->272 0.00100

135 ->228 -0.00118

136 ->175 0.00113

136 ->341 0.00116

137 ->197 -0.00106

137 ->236 0.00114

138 ->168 -0.00335

138 ->220 0.00119

138 ->256 -0.00103

138 ->325 -0.00102

139 ->202 0.00178

139 ->224 0.00168

139 ->238 0.00100

139 ->245 0.00114

140 ->168 0.00581

140 ->204 -0.00188

141 ->198 0.00133

141 ->222 -0.00119

141 ->253 -0.00105

142 ->185 0.00102

142 ->199 -0.00102

142 ->231 -0.00195

142 ->233 0.00113

143 ->203 0.00127

144 ->170 -0.00134

144 ->186 -0.00108

144 ->198 0.00127

144 ->210 -0.00127

144 ->253 -0.00101

145 ->231 -0.00156

145 ->244 -0.00104

146 ->171 0.00147

146 ->182 -0.00126

146 ->201 0.00112

146 ->207 -0.00115

146 ->223 0.00109

146 ->229 -0.00146

146 ->235 0.00133

146 ->237 0.00174

146 ->248 -0.00148

146 ->256 0.00205

146 ->269 0.00109

147 ->168 -0.01998

147 ->171 -0.00203

147 ->176 -0.00141

147 ->204 0.00207

147 ->212 0.00176

147 ->220 0.00213

147 ->265 0.00102

148 ->179 -0.00228

148 ->180 -0.00281

148 ->186 -0.00277

148 ->194 -0.00201

148 ->213 -0.00116

148 ->225 -0.00230

148 ->236 0.00210

148 ->250 0.00104

148 ->253 -0.00119

148 ->277 -0.00143

148 ->309 0.00109

148 ->317 0.00103

148 ->366 0.00130

148 ->378 -0.00121

149 ->169 -0.00138

149 ->226 -0.00164

149 ->240 -0.00113

150 ->174 0.00402

150 ->178 -0.00320

150 ->179 -0.01218

150 ->180 0.00394

150 ->190 -0.00187

150 ->197 0.00247

150 ->205 0.00610

150 ->216 0.00251

150 ->227 0.00169

150 ->274 0.00146

150 ->370 0.00121

151 ->169 -0.00265

151 ->189 0.00126

152 ->167 0.00279

152 ->172 0.00339

152 ->177 0.00170

152 ->184 0.00552

152 ->202 -0.00132

152 ->203 0.00369

152 ->208 -0.00115

152 ->211 0.00177

152 ->219 0.00180

153 ->167 -0.00158

153 ->172 0.00224

153 ->177 0.00131

153 ->184 -0.00371

153 ->203 -0.00178

153 ->219 -0.00107

153 ->224 -0.00111

153 ->245 0.00107

153 ->249 0.00135

153 ->272 -0.00163

154 ->167 -0.01082

154 ->172 0.00143

154 ->177 -0.00193

154 ->184 0.00135

154 ->203 0.00114

155 ->168 0.00727

155 ->171 0.00211

155 ->176 -0.00186

155 ->183 -0.00153

156 ->170 0.00203

156 ->174 -0.00306

156 ->179 0.00182

157 ->169 -0.00156

157 ->173 0.00245

157 ->175 -0.00195

158 ->167 0.01096

158 ->172 -0.00191

158 ->177 -0.00144

158 ->184 0.00258

158 ->219 0.00114

158 ->224 -0.00157

158 ->228 -0.00183

158 ->234 0.00123

158 ->238 0.00104

158 ->262 0.00143

158 ->272 -0.00105

159 ->168 -0.00503

159 ->171 -0.00595

159 ->176 -0.00228

159 ->207 0.00128

160 ->169 -0.00344

160 ->173 0.00141

160 ->175 0.00537

160 ->209 -0.00104

161 ->170 0.00311

161 ->174 -0.00178

161 ->179 0.01000

161 ->180 -0.00293

161 ->190 0.00109

161 ->205 -0.00289

161 ->216 -0.00211

161 ->227 -0.00137

161 ->236 -0.00156

161 ->283 -0.00100

162 ->169 -0.01640

162 ->173 0.00108

162 ->189 0.00344

163 ->170 0.00486

163 ->174 -0.00125

163 ->178 0.00310

163 ->210 0.00123

163 ->227 0.00182

164 ->167 0.03390

164 ->172 -0.00277

164 ->177 -0.00298

164 ->184 -0.00328

164 ->202 0.00119

164 ->203 -0.00381

164 ->211 -0.00121

164 ->219 -0.00221

165 ->168 -0.39512

165 ->171 -0.00284

165 ->176 -0.00693

165 ->183 0.01146

165 ->204 0.00319

165 ->207 -0.00115

165 ->212 0.00166

165 ->220 0.00230

165 ->248 -0.00106

166 ->167 0.58445

166 ->172 -0.00149

166 ->177 -0.00197

166 ->184 -0.00801

166 ->202 0.00175

166 ->203 -0.00739

166 ->211 -0.00305

166 ->218 -0.00176

166 ->219 -0.00549

166 ->266 -0.00194

166 ->336 0.00110

166 ->346 -0.00111

57 <-229 0.00107

58 <-225 -0.00121

58 <-232 0.00141

58 <-268 -0.00118

59 <-258 0.00100

60 <-228 0.00122

60 <-238 0.00122

72 <-229 0.00132

73 <-228 0.00135

73 <-238 0.00111

73 <-272 0.00103

74 <-236 -0.00142

74 <-317 -0.00125

75 <-226 -0.00107

75 <-231 -0.00105

75 <-258 0.00130

75 <-273 -0.00128

84 <-263 0.00108

85 <-323 0.00107

86 <-323 -0.00114

90 <-229 -0.00141

96 <-341 -0.00126

101 <-229 0.00126

104 <-226 0.00175

104 <-341 0.00167

104 <-347 -0.00112

106 <-168 -0.00129

106 <-248 0.00128

107 <-167 -0.00198

107 <-203 -0.00165

109 <-169 -0.00192

109 <-200 -0.00119

112 <-229 -0.00118

113 <-168 0.00132

113 <-235 0.00116

113 <-248 0.00121

113 <-256 -0.00146

113 <-321 -0.00106

113 <-325 -0.00123

113 <-350 0.00164

113 <-369 -0.00105

114 <-224 -0.00140

115 <-167 -0.00248

115 <-203 -0.00167

115 <-219 -0.00119

119 <-231 -0.00161

121 <-228 0.00108

121 <-238 0.00118

122 <-167 -0.00256

122 <-203 -0.00204

123 <-229 -0.00123

123 <-256 0.00140

124 <-169 -0.00393

124 <-200 -0.00247

124 <-221 -0.00117

125 <-205 0.00151

125 <-227 0.00134

126 <-240 -0.00111

126 <-258 0.00108

127 <-308 0.00100

127 <-317 0.00110

128 <-167 0.00198

129 <-229 -0.00116

130 <-324 -0.00132

132 <-317 0.00102

133 <-276 0.00107

133 <-285 0.00130

138 <-168 -0.00180

139 <-202 0.00117

139 <-224 0.00118

140 <-168 0.00318

140 <-204 -0.00168

142 <-231 -0.00140

145 <-231 -0.00113

146 <-229 -0.00111

146 <-237 0.00128

146 <-248 -0.00113

146 <-256 0.00157

147 <-168 -0.01052

147 <-183 -0.00175

147 <-204 0.00274

147 <-212 0.00160

147 <-220 0.00197

148 <-180 -0.00193

148 <-186 -0.00175

148 <-194 -0.00133

148 <-225 -0.00163

148 <-236 0.00155

148 <-277 -0.00115

148 <-366 0.00107

149 <-226 -0.00116

150 <-174 0.00117

150 <-178 -0.00218

150 <-179 -0.00355

150 <-180 0.00120

150 <-190 -0.00132

150 <-197 0.00180

150 <-205 0.00452

150 <-216 0.00186

150 <-227 0.00143

150 <-274 0.00123

150 <-370 0.00107

151 <-169 0.00524

151 <-189 0.00113

151 <-200 0.00103

152 <-172 0.00148

152 <-184 0.00336

152 <-203 0.00208

152 <-211 0.00103

153 <-167 0.00300

153 <-184 -0.00244

153 <-272 -0.00127

154 <-167 -0.00226

155 <-168 0.00198

156 <-174 -0.00125

156 <-179 0.00150

158 <-167 -0.00233

158 <-184 0.00226

158 <-228 -0.00120

158 <-262 0.00104

159 <-168 -0.00305

159 <-171 -0.00188

159 <-176 -0.00110

160 <-169 0.00128

160 <-175 0.00248

161 <-170 0.00109

161 <-179 0.00418

161 <-180 -0.00120

161 <-205 -0.00193

161 <-216 -0.00139

161 <-227 -0.00113

161 <-236 -0.00114

162 <-189 0.00200

163 <-170 0.00148

163 <-178 0.00206

163 <-179 -0.00337

163 <-180 0.00100

163 <-227 0.00116

164 <-167 0.00699

164 <-172 -0.00108

164 <-177 -0.00106

164 <-184 -0.00188

164 <-203 -0.00262

164 <-219 -0.00160

165 <-168 -0.02993

165 <-176 -0.00206

165 <-183 0.00601

165 <-204 0.00238

165 <-212 0.00103

165 <-220 0.00190

166 <-167 -0.01163

166 <-184 -0.00245

166 <-202 0.00106

166 <-203 -0.00415

166 <-211 -0.00220

166 <-219 -0.00316

166 <-266 -0.00163

Excited State 3: Singlet-E 3.0222 eV 410.25 nm f=1.6482 <S\*\*2>=0.000

58 ->226 0.00132

58 ->233 0.00111

58 ->280 -0.00102

59 ->222 -0.00110

60 ->223 -0.00105

64 ->223 -0.00110

70 ->233 0.00106

74 ->258 0.00127

74 ->285 -0.00112

75 ->222 -0.00175

75 ->236 -0.00113

76 ->202 -0.00128

76 ->224 -0.00121

76 ->245 -0.00104

76 ->251 -0.00117

76 ->270 -0.00107

77 ->168 0.00160

80 ->177 -0.00108

81 ->170 -0.00128

81 ->198 -0.00114

81 ->222 0.00120

82 ->206 -0.00123

82 ->285 0.00103

83 ->171 0.00134

83 ->201 -0.00109

84 ->208 -0.00158

84 ->211 -0.00101

84 ->224 0.00146

84 ->228 -0.00106

84 ->272 -0.00104

84 ->336 -0.00100

85 ->171 0.00132

85 ->229 -0.00251

86 ->223 -0.00175

86 ->229 0.00106

86 ->263 0.00103

87 ->196 0.00111

88 ->185 0.00105

88 ->199 -0.00132

88 ->206 -0.00200

88 ->209 0.00168

88 ->215 0.00127

88 ->247 0.00121

88 ->258 0.00175

88 ->264 0.00101

89 ->170 0.00200

89 ->222 0.00501

89 ->230 -0.00152

89 ->253 -0.00102

89 ->259 0.00116

89 ->268 0.00111

90 ->172 -0.00123

90 ->218 0.00121

90 ->224 0.00207

90 ->228 0.00125

90 ->272 0.00104

91 ->178 0.00118

91 ->179 -0.00109

91 ->205 -0.00161

91 ->227 0.00220

93 ->172 -0.00151

93 ->187 0.00119

93 ->202 0.00237

93 ->208 0.00339

93 ->218 0.00137

93 ->224 0.00490

93 ->238 -0.00266

93 ->262 -0.00153

93 ->349 -0.00103

94 ->224 -0.00102

94 ->228 0.00104

94 ->234 -0.00151

94 ->238 -0.00205

94 ->245 -0.00109

94 ->249 -0.00112

94 ->270 -0.00130

94 ->272 0.00119

95 ->185 -0.00117

95 ->226 -0.00169

95 ->231 -0.00139

95 ->258 -0.00117

96 ->180 -0.00276

96 ->190 0.00104

96 ->194 0.00110

96 ->197 0.00209

96 ->198 0.00146

96 ->232 -0.00284

96 ->239 0.00187

96 ->259 0.00168

96 ->260 0.00119

96 ->268 0.00157

97 ->192 -0.00200

97 ->196 -0.00272

97 ->223 0.00219

97 ->237 0.00178

97 ->263 -0.00105

98 ->182 -0.00116

98 ->188 0.00158

98 ->196 -0.00110

98 ->235 -0.00103

99 ->199 0.00120

99 ->206 0.00168

99 ->209 -0.00128

99 ->215 -0.00115

99 ->226 -0.00283

99 ->231 0.00176

99 ->233 -0.00151

99 ->247 -0.00174

99 ->258 -0.00234

99 ->341 0.00121

100 ->170 -0.00102

100 ->179 -0.00166

100 ->180 -0.00465

100 ->186 -0.00340

100 ->190 0.00238

100 ->194 0.00293

100 ->197 0.00337

100 ->198 0.00212

100 ->216 0.00117

100 ->225 -0.00279

100 ->230 0.00163

100 ->239 0.00105

100 ->250 -0.00114

100 ->253 0.00172

100 ->261 -0.00121

101 ->172 0.00120

101 ->181 0.00146

101 ->187 -0.00202

101 ->218 -0.00153

101 ->224 -0.00156

101 ->245 -0.00195

101 ->249 -0.00137

101 ->251 -0.00123

101 ->257 0.00144

102 ->182 0.00176

102 ->192 0.00345

102 ->196 0.00479

102 ->201 0.00103

102 ->223 0.00186

102 ->237 -0.00340

102 ->248 -0.00178

102 ->256 0.00170

103 ->185 -0.00173

103 ->231 0.00155

103 ->233 -0.00174

104 ->180 -0.00233

104 ->186 0.00150

104 ->222 0.00172

104 ->225 -0.00326

104 ->230 -0.00300

104 ->232 0.00286

104 ->236 0.00138

104 ->239 -0.00274

104 ->250 -0.00162

104 ->260 -0.00159

104 ->268 -0.00125

105 ->171 0.00127

105 ->217 -0.00260

105 ->220 -0.00107

105 ->223 -0.00103

105 ->246 -0.00178

106 ->167 0.00177

106 ->184 0.00105

106 ->218 0.00120

106 ->219 0.00128

106 ->228 0.00301

106 ->245 0.00154

106 ->249 0.00205

106 ->257 -0.00115

106 ->272 0.00173

107 ->168 0.00509

107 ->248 -0.00151

108 ->169 0.00268

108 ->200 0.00103

108 ->233 -0.00103

108 ->254 0.00127

109 ->170 0.00139

109 ->178 -0.00128

109 ->179 0.00161

109 ->216 -0.00138

109 ->230 -0.00102

109 ->236 0.00113

109 ->255 0.00130

110 ->169 0.00116

110 ->175 0.00195

110 ->199 -0.00118

110 ->214 -0.00165

110 ->221 0.00127

110 ->226 0.00122

110 ->254 0.00105

111 ->170 0.00188

111 ->179 -0.00137

111 ->198 0.00169

111 ->213 -0.00165

111 ->216 -0.00186

111 ->230 -0.00277

111 ->232 0.00226

111 ->236 0.00124

111 ->253 -0.00112

111 ->255 -0.00111

111 ->260 -0.00108

111 ->308 -0.00110

111 ->309 0.00117

112 ->172 -0.00197

112 ->187 0.00173

112 ->219 0.00219

112 ->234 0.00116

112 ->249 0.00184

112 ->257 -0.00159

113 ->167 -0.00176

113 ->187 0.00111

113 ->203 -0.00130

113 ->208 -0.00140

113 ->211 -0.00136

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111 <-198 0.00107

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111 <-232 0.00165

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113 <-249 0.00111

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113 <-336 0.00116

114 <-188 0.00164

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114 <-196 0.00176

114 <-223 0.00251

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117 <-178 -0.00105

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119 <-230 0.00160

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159 <-172 -0.00323

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165 <-172 0.00191

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166 <-168 0.09153

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166 <-176 0.00850

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166 <-212 -0.00272

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166 <-339 -0.00114

Excited State 4: Singlet-E 3.0222 eV 410.25 nm f=1.6482 <S\*\*2>=0.000

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74 ->222 -0.00175

74 ->236 0.00113

75 ->258 0.00127

75 ->285 0.00112

76 ->201 0.00128

76 ->223 0.00121

76 ->246 0.00104

76 ->252 0.00117

76 ->269 0.00107

77 ->167 -0.00160

80 ->176 -0.00108

81 ->206 0.00123

81 ->285 0.00103

82 ->170 -0.00128

82 ->198 0.00114

82 ->222 -0.00120

83 ->172 -0.00134

83 ->202 0.00109

84 ->207 0.00158

84 ->212 0.00101

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84 ->229 0.00106

84 ->271 -0.00104

84 ->335 0.00100

85 ->172 0.00132

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136 <-275 -0.00107

137 <-170 -0.00138

137 <-180 0.00243

137 <-186 0.00112

137 <-194 -0.00125

137 <-198 -0.00132

137 <-222 0.00286

137 <-225 0.00197

137 <-230 0.00110

137 <-232 -0.00180

137 <-236 0.00146

137 <-268 0.00116

138 <-176 0.00132

138 <-183 -0.00103

138 <-196 -0.00219

138 <-207 0.00173

138 <-212 0.00108

138 <-223 -0.00395

138 <-229 0.00352

138 <-237 0.00118

138 <-246 0.00101

138 <-263 0.00119

138 <-279 -0.00191

138 <-294 -0.00107

139 <-202 0.00211

139 <-224 0.00213

139 <-238 0.00112

139 <-245 0.00167

140 <-183 0.00137

140 <-223 -0.00126

140 <-229 0.00118

140 <-242 -0.00115

141 <-170 -0.00149

141 <-213 0.00104

141 <-216 0.00157

141 <-230 0.00271

141 <-232 -0.00132

141 <-241 -0.00115

141 <-253 -0.00113

142 <-185 0.00110

142 <-199 -0.00126

142 <-206 0.00139

142 <-226 0.00139

142 <-231 -0.00239

142 <-233 0.00120

143 <-167 0.00344

143 <-203 0.00121

143 <-243 0.00119

144 <-178 0.00101

144 <-186 -0.00116

144 <-198 0.00150

144 <-210 -0.00152

144 <-230 0.00181

144 <-253 -0.00125

145 <-200 -0.00102

145 <-231 -0.00141

145 <-244 -0.00109

146 <-171 0.00209

146 <-182 -0.00129

146 <-207 -0.00198

146 <-220 -0.00112

146 <-235 0.00120

146 <-237 0.00163

146 <-248 -0.00268

146 <-256 0.00303

146 <-269 0.00149

146 <-271 -0.00109

146 <-297 -0.00144

146 <-310 -0.00130

147 <-171 -0.00207

147 <-183 -0.00297

147 <-204 -0.00194

147 <-212 0.00132

147 <-265 0.00192

147 <-282 -0.00139

147 <-294 -0.00109

148 <-170 0.00109

148 <-179 -0.00407

148 <-180 -0.00848

148 <-186 -0.00666

148 <-190 0.00106

148 <-194 -0.00456

148 <-197 0.00105

148 <-198 0.00176

148 <-213 -0.00212

148 <-222 0.00173

148 <-225 -0.00593

148 <-232 -0.00112

148 <-236 0.00167

148 <-239 0.00277

148 <-250 0.00257

148 <-253 -0.00217

148 <-260 0.00175

148 <-261 0.00116

148 <-277 0.00183

148 <-283 0.00107

148 <-476 0.00129

149 <-175 0.00109

149 <-226 -0.00514

149 <-231 -0.00327

149 <-233 0.00119

149 <-240 -0.00105

149 <-258 -0.00136

149 <-264 -0.00262

149 <-273 -0.00289

149 <-280 0.00223

149 <-292 0.00146

149 <-329 -0.00107

149 <-341 0.00158

149 <-343 0.00123

150 <-170 -0.00121

150 <-178 -0.00159

150 <-179 0.00155

150 <-205 0.00240

150 <-255 0.00124

150 <-283 -0.00123

150 <-284 0.00121

150 <-289 0.00136

150 <-309 0.00141

151 <-173 0.00321

151 <-185 0.00136

151 <-189 0.00508

151 <-200 -0.00147

151 <-209 0.00126

151 <-215 -0.00109

151 <-267 0.00188

151 <-275 -0.00102

151 <-302 -0.00120

152 <-167 0.01584

152 <-172 0.00216

152 <-184 -0.00107

152 <-195 0.00103

152 <-208 -0.00135

152 <-219 -0.00104

152 <-238 0.00151

152 <-245 -0.00110

152 <-281 -0.00117

152 <-288 -0.00101

153 <-167 0.00355

153 <-172 0.00326

153 <-184 -0.00236

153 <-187 -0.00127

153 <-191 0.00106

153 <-202 -0.00190

153 <-208 -0.00139

153 <-211 0.00123

153 <-218 -0.00146

153 <-228 -0.00411

153 <-238 0.00351

153 <-249 0.00111

153 <-266 0.00116

153 <-272 -0.00315

153 <-278 0.00141

153 <-281 0.00104

153 <-301 -0.00111

153 <-305 0.00148

153 <-311 0.00115

153 <-323 0.00128

153 <-334 -0.00131

154 <-177 -0.00245

154 <-184 -0.00180

155 <-168 0.00621

155 <-171 0.00277

156 <-170 0.00282

156 <-174 -0.00112

156 <-178 -0.00251

156 <-197 0.00131

156 <-205 0.00148

157 <-169 0.00142

157 <-173 0.00353

157 <-189 0.00169

157 <-200 0.00113

158 <-172 -0.00209

158 <-177 0.00151

158 <-181 -0.00198

158 <-184 0.00127

158 <-187 -0.00156

158 <-203 -0.00190

158 <-218 -0.00126

158 <-228 -0.00468

158 <-234 0.00253

158 <-238 0.00379

158 <-249 0.00242

158 <-272 -0.00528

158 <-288 -0.00107

158 <-334 -0.00154

158 <-338 -0.00104

159 <-171 -0.00323

159 <-176 -0.00339

159 <-196 0.00119

159 <-204 -0.00200

159 <-212 -0.00114

159 <-235 -0.00130

159 <-252 -0.00111

159 <-271 0.00119

159 <-335 -0.00121

160 <-175 0.00517

160 <-200 -0.00330

160 <-206 0.00131

161 <-170 0.00298

161 <-174 0.00322

161 <-178 -0.00332

161 <-190 -0.00171

161 <-194 0.00104

161 <-205 0.00162

161 <-227 -0.00123

161 <-232 0.00105

161 <-289 -0.00141

161 <-309 -0.00121

161 <-318 -0.00116

162 <-169 -0.00701

162 <-173 0.00214

162 <-175 -0.00119

162 <-185 0.00127

162 <-189 0.00655

162 <-200 0.00152

162 <-221 0.00164

162 <-226 0.00102

162 <-273 -0.00114

162 <-312 0.00116

162 <-326 -0.00128

163 <-170 0.00287

163 <-178 0.00743

163 <-179 0.00332

163 <-180 -0.00133

163 <-190 0.00212

163 <-197 -0.00216

163 <-205 -0.00309

163 <-210 0.00241

163 <-216 -0.00212

163 <-227 0.00355

163 <-274 -0.00135

163 <-283 -0.00132

163 <-299 -0.00118

163 <-309 0.00109

163 <-330 -0.00150

163 <-332 0.00133

164 <-172 -0.00190

164 <-177 -0.00145

164 <-184 0.00717

164 <-203 -0.00134

164 <-288 0.00110

164 <-305 0.00187

164 <-311 0.00153

164 <-315 0.00217

165 <-168 -0.08030

165 <-171 -0.00191

165 <-176 -0.00732

165 <-183 0.00792

165 <-204 0.00340

165 <-220 0.00184

165 <-248 -0.00156

165 <-252 0.00127

165 <-279 0.00134

165 <-300 -0.00105

165 <-325 -0.00149

165 <-333 0.00130

165 <-339 0.00188

165 <-345 0.00124

166 <-167 -0.09153

166 <-172 0.00324

166 <-177 0.00850

166 <-184 0.01321

166 <-195 0.00118

166 <-203 -0.00191

166 <-211 -0.00272

166 <-219 -0.00324

166 <-224 0.00126

166 <-249 0.00152

166 <-266 -0.00197

166 <-281 0.00158

166 <-288 0.00137

166 <-295 0.00105

166 <-305 0.00116

166 <-338 0.00114

Excited State 5: Singlet-E 3.5769 eV 346.62 nm f=0.0000 <S\*\*2>=0.000

62 ->208 0.00108

63 ->207 -0.00108

64 ->206 -0.00123

74 ->229 0.00109

75 ->228 0.00109

84 ->190 -0.00142

84 ->197 -0.00188

84 ->261 0.00134

85 ->226 0.00149

85 ->231 0.00136

85 ->233 -0.00112

86 ->226 -0.00114

86 ->231 -0.00142

86 ->233 0.00117

88 ->182 0.00101

88 ->196 0.00144

88 ->229 0.00155

89 ->181 -0.00101

89 ->195 -0.00144

89 ->228 -0.00155

93 ->180 -0.00177

93 ->194 0.00173

93 ->222 0.00194

93 ->277 0.00101

95 ->229 0.00126

96 ->228 -0.00126

97 ->209 -0.00101

99 ->207 -0.00108

99 ->223 0.00156

100 ->208 0.00108

100 ->224 -0.00156

102 ->206 -0.00157

102 ->258 -0.00153

102 ->401 0.00107

103 ->223 0.00128

103 ->229 -0.00145

104 ->224 -0.00128

104 ->228 0.00145

106 ->222 -0.00163

108 ->168 0.00201

109 ->167 -0.00201

110 ->168 0.00154

111 ->167 0.00154

113 ->186 -0.00105

113 ->222 -0.00284

113 ->253 0.00118

114 ->169 0.00123

114 ->240 0.00179

114 ->244 -0.00112

114 ->390 0.00106

115 ->189 0.00126

116 ->168 0.00253

117 ->167 -0.00253

119 ->167 -0.00240

119 ->228 -0.00115

119 ->234 0.00129

120 ->168 -0.00240

120 ->229 0.00115

120 ->235 -0.00129

121 ->240 0.00246

121 ->244 -0.00199

121 ->254 0.00133

121 ->276 -0.00225

121 ->293 -0.00123

121 ->355 -0.00121

121 ->390 0.00167

121 ->441 -0.00101

122 ->189 0.00115

123 ->190 -0.00105

123 ->197 -0.00145

124 ->167 -0.01781

124 ->177 0.00206

124 ->184 -0.00186

124 ->203 -0.00101

125 ->168 0.01781

125 ->176 0.00206

125 ->183 0.00186

125 ->204 -0.00101

126 ->167 0.00202

126 ->224 -0.00146

126 ->234 0.00111

126 ->278 -0.00123

127 ->168 0.00202

127 ->223 0.00146

127 ->235 -0.00111

127 ->279 0.00123

128 ->169 0.01587

128 ->175 0.00492

128 ->193 -0.00118

128 ->200 0.00173

129 ->261 0.00140

130 ->226 -0.00367

130 ->264 0.00116

130 ->292 -0.00116

130 ->296 -0.00144

130 ->343 -0.00193

130 ->362 -0.00160

130 ->387 -0.00106

130 ->422 -0.00102

131 ->180 -0.00122

131 ->277 0.00149

132 ->229 0.00158

132 ->271 0.00106

132 ->279 0.00118

132 ->333 -0.00119

132 ->335 0.00100

132 ->389 0.00101

133 ->228 -0.00158

133 ->272 0.00106

133 ->278 -0.00118

133 ->334 0.00119

133 ->336 -0.00100

133 ->388 -0.00101

134 ->206 0.00125

134 ->226 -0.00138

134 ->343 -0.00123

134 ->362 -0.00116

135 ->169 -0.00310

135 ->240 -0.00146

135 ->244 0.00124

136 ->195 -0.00112

137 ->196 0.00112

138 ->194 0.00188

138 ->222 -0.00119

138 ->277 -0.00121

141 ->168 -0.00177

142 ->167 -0.00177

144 ->168 0.00376

145 ->167 0.00376

146 ->170 0.00123

147 ->174 0.00166

147 ->179 -0.00264

148 ->223 0.00179

148 ->229 0.00112

148 ->235 -0.00103

149 ->224 -0.00179

149 ->228 -0.00112

149 ->234 0.00103

150 ->168 -0.03062

150 ->171 -0.00223

150 ->183 -0.00391

151 ->167 -0.03062

151 ->172 0.00223

151 ->184 -0.00391

152 ->173 0.00288

152 ->185 0.00154

152 ->189 0.00733

152 ->206 -0.00220

152 ->273 0.00102

153 ->173 -0.00110

153 ->185 -0.00147

153 ->189 -0.00740

153 ->226 -0.00208

154 ->169 -0.01684

154 ->175 0.00163

154 ->193 0.00143

154 ->200 -0.00551

154 ->209 -0.00102

154 ->221 -0.00193

155 ->170 0.00272

156 ->168 -0.05842

156 ->171 0.00261

156 ->183 0.00320

156 ->204 0.00210

156 ->220 0.00101

157 ->167 -0.05842

157 ->172 -0.00261

157 ->184 0.00320

157 ->203 -0.00210

157 ->219 -0.00101

158 ->173 0.00110

158 ->189 0.00668

158 ->226 -0.00153

158 ->343 -0.00124

158 ->362 -0.00100

159 ->179 -0.00527

159 ->180 0.00253

159 ->194 -0.00152

159 ->222 0.00117

160 ->167 0.10616

160 ->177 -0.00190

160 ->184 -0.00719

160 ->195 -0.00133

160 ->203 0.00381

160 ->211 0.00188

160 ->219 0.00258

160 ->224 -0.00121

161 ->168 -0.10616

161 ->176 -0.00190

161 ->183 0.00719

161 ->196 -0.00133

161 ->204 0.00381

161 ->212 0.00188

161 ->220 0.00258

161 ->223 -0.00121

162 ->167 -0.48132

162 ->177 0.00904

162 ->181 -0.00101

162 ->184 0.01177

162 ->202 0.00111

162 ->203 -0.00598

162 ->208 0.00213

162 ->211 -0.00228

162 ->218 -0.00138

162 ->219 -0.00396

162 ->249 0.00158

162 ->315 -0.00105

163 ->168 0.48132

163 ->176 0.00904

163 ->182 -0.00101

163 ->183 -0.01177

163 ->201 0.00111

163 ->204 -0.00598

163 ->207 0.00213

163 ->212 -0.00228

163 ->217 -0.00138

163 ->220 -0.00396

163 ->248 0.00158

163 ->316 -0.00105

164 ->169 0.05331

164 ->175 0.00397

164 ->193 -0.00317

164 ->200 0.01587

164 ->209 0.00134

164 ->215 -0.00347

164 ->221 0.00614

164 ->254 -0.00153

164 ->267 0.00145

164 ->326 0.00197

165 ->170 0.00245

165 ->178 -0.00563

165 ->205 0.00296

165 ->210 0.00144

165 ->227 0.00156

165 ->289 0.00103

165 ->309 0.00106

165 ->492 0.00115

166 ->189 -0.00627

84 <-197 -0.00121

85 <-226 0.00104

85 <-231 0.00102

86 <-231 -0.00101

88 <-229 0.00102

89 <-228 -0.00102

93 <-180 -0.00107

93 <-194 0.00110

93 <-222 0.00126

99 <-223 0.00100

100 <-224 -0.00100

102 <-206 -0.00101

102 <-258 -0.00102

113 <-222 -0.00172

114 <-240 0.00121

121 <-240 0.00165

121 <-244 -0.00133

121 <-276 -0.00167

121 <-390 0.00133

124 <-167 -0.00414

124 <-184 -0.00147

125 <-168 0.00414

125 <-183 0.00147

128 <-169 0.00511

128 <-175 0.00188

130 <-226 -0.00227

130 <-296 -0.00105

130 <-343 -0.00144

130 <-362 -0.00122

132 <-229 0.00112

133 <-228 -0.00112

147 <-179 0.00140

150 <-168 -0.00453

150 <-183 -0.00314

151 <-167 -0.00453

151 <-184 -0.00314

152 <-173 0.00103

152 <-189 0.00481

152 <-206 -0.00133

152 <-273 0.00103

153 <-189 -0.00498

154 <-169 0.00272

154 <-175 0.00220

154 <-200 -0.00140

156 <-168 0.00161

156 <-183 0.00166

157 <-167 0.00161

157 <-184 0.00166

158 <-189 0.00422

158 <-343 -0.00107

160 <-167 -0.00529

160 <-184 -0.00412

161 <-168 0.00529

161 <-183 0.00412

162 <-167 0.00555

162 <-172 -0.00123

162 <-184 0.00458

162 <-203 -0.00212

162 <-219 -0.00188

163 <-168 -0.00555

163 <-171 -0.00123

163 <-183 -0.00458

163 <-204 -0.00212

163 <-220 -0.00188

164 <-169 -0.00899

164 <-175 -0.00401

164 <-200 0.00361

164 <-215 -0.00107

164 <-221 0.00224

164 <-312 -0.00109

164 <-326 0.00101

165 <-178 -0.00368

165 <-197 0.00114

165 <-205 0.00239

165 <-216 0.00127

165 <-492 0.00109

Excited State 6: Singlet-E 3.6197 eV 342.53 nm f=0.0000 <S\*\*2>=0.000

60 ->226 0.00103

61 ->206 -0.00166

61 ->231 -0.00142

61 ->247 0.00136

61 ->258 0.00146

61 ->280 0.00105

61 ->422 -0.00106

62 ->208 -0.00136

63 ->207 -0.00136

64 ->209 -0.00117

64 ->215 -0.00107

64 ->275 0.00102

74 ->229 0.00189

75 ->228 -0.00189

81 ->224 0.00137

82 ->223 0.00137

84 ->180 -0.00158

84 ->194 0.00156

84 ->222 0.00374

84 ->225 0.00102

84 ->232 -0.00129

84 ->268 0.00159

84 ->277 0.00184

85 ->240 -0.00173

85 ->244 0.00116

85 ->276 0.00103

86 ->240 0.00103

87 ->226 0.00126

88 ->182 -0.00101

88 ->196 -0.00123

88 ->223 0.00307

89 ->181 -0.00101

89 ->195 -0.00123

89 ->224 0.00307

93 ->190 -0.00168

93 ->197 -0.00211

93 ->216 -0.00103

93 ->230 -0.00282

93 ->261 0.00152

93 ->317 -0.00118

93 ->406 -0.00104

94 ->222 -0.00117

95 ->235 -0.00119

95 ->279 0.00120

96 ->234 -0.00119

96 ->278 0.00120

97 ->206 -0.00141

97 ->226 -0.00214

97 ->258 -0.00128

97 ->264 0.00105

97 ->401 0.00110

99 ->182 0.00103

99 ->196 0.00127

99 ->207 -0.00138

99 ->304 -0.00107

100 ->181 0.00103

100 ->195 0.00127

100 ->208 -0.00138

100 ->305 0.00107

102 ->209 -0.00147

102 ->215 -0.00113

102 ->312 0.00103

102 ->329 -0.00106

102 ->341 0.00171

102 ->390 -0.00157

103 ->246 0.00114

103 ->279 -0.00105

104 ->245 0.00114

104 ->278 -0.00105

106 ->236 0.00108

106 ->317 0.00100

107 ->169 0.00364

107 ->175 0.00119

108 ->168 0.00309

109 ->167 0.00309

110 ->168 0.00188

111 ->167 -0.00188

113 ->230 -0.00123

113 ->236 0.00155

113 ->255 -0.00100

113 ->309 0.00130

113 ->317 0.00155

114 ->185 -0.00105

114 ->226 -0.00191

114 ->264 0.00107

114 ->343 -0.00114

115 ->169 0.00507

115 ->175 0.00286

115 ->200 -0.00114

116 ->168 0.00178

116 ->196 0.00105

117 ->167 0.00178

117 ->195 -0.00105

118 ->190 0.00106

119 ->167 0.00275

119 ->191 0.00128

119 ->224 0.00132

119 ->278 0.00117

120 ->168 -0.00275

120 ->192 0.00128

120 ->223 0.00132

120 ->279 0.00117

121 ->199 0.00131

121 ->206 0.00163

121 ->226 -0.00242

121 ->231 -0.00114

121 ->296 -0.00151

121 ->343 -0.00232

121 ->362 -0.00215

121 ->387 -0.00130

121 ->422 -0.00102

121 ->444 -0.00100

122 ->169 0.00533

122 ->175 0.00277

122 ->193 -0.00103

122 ->200 -0.00102

123 ->194 0.00309

123 ->222 -0.00197

123 ->277 -0.00209

123 ->378 -0.00101

124 ->167 0.01283

124 ->172 -0.00203

124 ->177 -0.00154

124 ->184 0.00376

124 ->191 -0.00104

125 ->168 0.01283

125 ->171 0.00203

125 ->176 0.00154

125 ->183 0.00376

125 ->192 0.00104

126 ->167 -0.00132

126 ->202 0.00114

126 ->224 0.00112

126 ->228 0.00152

126 ->334 -0.00121

126 ->336 0.00143

126 ->377 0.00107

127 ->168 0.00132

127 ->201 0.00114

127 ->223 0.00112

127 ->229 0.00152

127 ->333 -0.00121

127 ->335 0.00143

127 ->376 0.00107

128 ->185 0.00111

128 ->189 0.00676

128 ->206 -0.00112

129 ->194 -0.00164

129 ->198 -0.00104

129 ->222 0.00239

129 ->225 -0.00101

129 ->330 -0.00127

129 ->378 0.00107

130 ->169 -0.00124

130 ->175 0.00137

130 ->215 0.00117

130 ->240 0.00227

130 ->244 -0.00194

130 ->254 0.00121

130 ->276 -0.00188

130 ->285 0.00104

130 ->329 -0.00160

130 ->341 0.00138

130 ->355 -0.00116

130 ->390 0.00147

130 ->421 -0.00115

130 ->441 -0.00128

131 ->230 -0.00165

131 ->261 0.00143

131 ->274 -0.00116

131 ->284 0.00122

131 ->289 -0.00111

131 ->317 -0.00102

132 ->196 -0.00129

132 ->207 0.00118

132 ->223 -0.00157

132 ->229 0.00211

132 ->304 -0.00144

132 ->316 -0.00145

133 ->195 -0.00129

133 ->208 0.00118

133 ->224 -0.00157

133 ->228 0.00211

133 ->305 0.00144

133 ->315 -0.00145

134 ->169 0.00196

134 ->209 0.00170

134 ->215 0.00116

134 ->390 0.00122

135 ->189 -0.00120

135 ->231 -0.00167

135 ->264 -0.00179

135 ->273 -0.00129

135 ->280 0.00172

135 ->343 0.00163

136 ->167 0.00310

136 ->172 0.00133

136 ->191 -0.00134

136 ->195 -0.00163

136 ->224 -0.00128

136 ->228 0.00126

137 ->168 -0.00310

137 ->171 0.00133

137 ->192 -0.00134

137 ->196 -0.00163

137 ->223 -0.00128

137 ->229 0.00126

138 ->170 -0.00115

138 ->190 -0.00139

138 ->197 -0.00223

138 ->230 0.00169

138 ->236 0.00164

138 ->261 -0.00132

138 ->317 0.00124

138 ->374 -0.00130

139 ->199 -0.00118

139 ->231 -0.00125

140 ->210 0.00109

141 ->256 0.00110

142 ->257 0.00110

143 ->200 -0.00141

144 ->204 0.00106

145 ->203 0.00106

146 ->198 0.00119

146 ->260 -0.00126

146 ->330 -0.00122

146 ->332 -0.00108

147 ->170 0.00326

147 ->205 -0.00126

148 ->263 -0.00119

148 ->271 0.00167

148 ->304 -0.00131

148 ->316 -0.00136

148 ->333 -0.00134

148 ->350 0.00107

148 ->369 -0.00121

149 ->262 -0.00119

149 ->272 -0.00167

149 ->305 0.00131

149 ->315 -0.00136

149 ->334 -0.00134

149 ->349 0.00107

149 ->368 -0.00121

150 ->168 0.02921

150 ->176 0.00158

150 ->183 -0.00537

150 ->204 -0.00285

150 ->207 0.00165

150 ->212 -0.00176

150 ->217 -0.00119

150 ->220 -0.00284

150 ->265 -0.00112

150 ->282 0.00119

151 ->167 -0.02921

151 ->177 0.00158

151 ->184 0.00537

151 ->203 -0.00285

151 ->208 0.00165

151 ->211 -0.00176

151 ->218 -0.00119

151 ->219 -0.00284

151 ->266 -0.00112

151 ->281 0.00119

152 ->169 -0.03991

152 ->175 -0.00224

152 ->193 0.00198

152 ->200 -0.01065

152 ->209 -0.00272

152 ->215 0.00230

152 ->221 -0.00432

152 ->254 0.00106

152 ->267 -0.00137

152 ->326 -0.00137

153 ->169 0.02714

153 ->175 0.00475

153 ->193 -0.00153

153 ->200 0.00733

153 ->215 -0.00172

153 ->221 0.00340

153 ->326 0.00178

153 ->329 -0.00206

153 ->341 0.00167

154 ->189 0.00274

154 ->206 -0.00180

155 ->194 -0.00136

156 ->168 -0.04750

156 ->171 -0.00118

156 ->176 -0.00162

156 ->183 0.00270

156 ->196 0.00111

157 ->167 0.04750

157 ->172 -0.00118

157 ->177 -0.00162

157 ->184 -0.00270

157 ->195 0.00111

158 ->169 -0.02146

158 ->175 -0.00268

158 ->193 0.00109

158 ->200 -0.00574

158 ->215 0.00188

158 ->221 -0.00247

158 ->254 0.00100

158 ->267 -0.00161

158 ->312 0.00101

158 ->326 -0.00103

158 ->341 0.00194

159 ->170 0.00611

159 ->197 0.00255

159 ->205 0.00164

159 ->236 -0.00140

160 ->167 -0.16127

160 ->172 0.00347

160 ->177 0.00497

160 ->184 0.00752

160 ->203 -0.00231

160 ->211 -0.00135

160 ->219 -0.00245

160 ->249 0.00102

160 ->315 -0.00125

161 ->168 -0.16127

161 ->171 -0.00347

161 ->176 -0.00497

161 ->183 0.00752

161 ->204 0.00231

161 ->212 0.00135

161 ->220 0.00245

161 ->248 -0.00102

161 ->316 0.00125

162 ->167 0.46206

162 ->172 0.00303

162 ->177 -0.00516

162 ->184 -0.00533

162 ->195 -0.00120

162 ->202 -0.00146

162 ->203 0.00504

162 ->208 -0.00222

162 ->211 0.00215

162 ->219 0.00274

162 ->305 0.00105

162 ->315 0.00126

163 ->168 0.46206

163 ->171 -0.00303

163 ->176 0.00516

163 ->183 -0.00533

163 ->196 0.00120

163 ->201 0.00146

163 ->204 -0.00504

163 ->207 0.00222

163 ->212 -0.00215

163 ->220 -0.00274

163 ->304 0.00105

163 ->316 -0.00126

164 ->173 -0.00131

164 ->185 -0.00114

164 ->189 -0.00753

164 ->206 0.00102

164 ->495 -0.00142

165 ->174 -0.00542

165 ->179 0.01405

165 ->180 -0.00366

165 ->283 -0.00107

165 ->330 -0.00111

165 ->332 0.00129

166 ->169 -0.10157

166 ->200 0.00532

166 ->215 -0.00257

166 ->221 0.00434

166 ->267 0.00212

166 ->275 -0.00126

166 ->329 -0.00126

61 <-206 -0.00120

61 <-231 -0.00116

61 <-247 0.00104

61 <-258 0.00107

74 <-229 0.00132

75 <-228 -0.00132

84 <-194 0.00103

84 <-222 0.00246

84 <-277 0.00125

85 <-240 -0.00120

88 <-223 0.00205

89 <-224 0.00205

93 <-190 -0.00101

93 <-197 -0.00132

93 <-230 -0.00201

93 <-261 0.00104

97 <-226 -0.00142

102 <-341 0.00127

102 <-390 -0.00121

107 <-169 0.00215

108 <-168 0.00132

109 <-167 0.00132

113 <-236 0.00114

113 <-317 0.00114

114 <-226 -0.00122

115 <-169 0.00274

115 <-175 0.00142

115 <-200 -0.00106

121 <-226 -0.00155

121 <-296 -0.00114

121 <-343 -0.00173

121 <-362 -0.00165

121 <-387 -0.00102

122 <-169 0.00250

122 <-175 0.00127

122 <-200 -0.00102

123 <-194 0.00164

123 <-222 -0.00105

123 <-277 -0.00143

124 <-167 0.00309

124 <-184 0.00324

125 <-168 0.00309

125 <-183 0.00324

126 <-228 0.00105

126 <-336 0.00107

127 <-229 0.00105

127 <-335 0.00107

128 <-189 0.00457

129 <-222 0.00137

130 <-240 0.00145

130 <-244 -0.00124

130 <-276 -0.00137

130 <-329 -0.00116

130 <-390 0.00115

130 <-441 -0.00103

132 <-229 0.00128

133 <-228 0.00128

135 <-231 -0.00105

135 <-264 -0.00121

135 <-280 0.00112

135 <-343 0.00120

138 <-197 -0.00117

147 <-205 -0.00136

148 <-271 0.00107

149 <-272 -0.00107

150 <-168 0.00526

150 <-183 -0.00286

150 <-204 -0.00116

150 <-212 -0.00105

150 <-220 -0.00149

151 <-167 -0.00526

151 <-184 0.00286

151 <-203 -0.00116

151 <-211 -0.00105

151 <-219 -0.00149

152 <-169 0.00368

152 <-175 0.00202

152 <-200 -0.00241

152 <-209 -0.00116

152 <-221 -0.00154

152 <-267 -0.00100

153 <-169 -0.00598

153 <-175 -0.00192

153 <-221 0.00113

153 <-329 -0.00162

153 <-341 0.00114

154 <-189 0.00202

156 <-168 0.00247

156 <-183 0.00147

157 <-167 -0.00247

157 <-184 -0.00147

158 <-169 0.00447

158 <-175 0.00182

158 <-267 -0.00104

158 <-341 0.00137

160 <-167 0.00164

160 <-184 0.00343

161 <-168 0.00164

161 <-183 0.00343

162 <-167 -0.01085

162 <-177 0.00118

162 <-184 -0.00352

163 <-168 -0.01085

163 <-176 -0.00118

163 <-183 -0.00352

164 <-189 -0.00578

164 <-273 -0.00115

164 <-296 -0.00128

165 <-179 0.00600

165 <-180 -0.00180

166 <-169 0.01021

166 <-175 0.00197

166 <-200 0.00355

166 <-215 -0.00151

166 <-221 0.00208

166 <-267 0.00143

Excited State 7: Singlet-E 3.6414 eV 340.48 nm f=0.0464 <S\*\*2>=0.000

50 ->230 0.00102

52 ->223 -0.00126

61 ->207 -0.00116

61 ->237 0.00114

62 ->180 -0.00127

63 ->206 -0.00121

74 ->240 0.00103

84 ->181 -0.00111

84 ->191 -0.00112

84 ->195 -0.00146

84 ->224 0.00143

84 ->228 -0.00101

85 ->279 -0.00112

88 ->206 -0.00116

88 ->240 0.00146

88 ->244 -0.00121

89 ->190 -0.00108

89 ->194 0.00170

89 ->197 -0.00133

89 ->222 0.00110

89 ->230 -0.00102

93 ->181 -0.00134

93 ->191 -0.00112

93 ->195 -0.00193

93 ->224 0.00105

93 ->234 -0.00105

93 ->270 -0.00135

95 ->226 -0.00133

96 ->180 0.00127

96 ->194 0.00120

97 ->207 -0.00114

97 ->229 0.00147

99 ->206 -0.00110

99 ->209 -0.00145

99 ->215 -0.00102

99 ->390 -0.00102

99 ->401 0.00106

100 ->179 0.00106

100 ->180 0.00231

100 ->186 0.00172

100 ->190 0.00104

100 ->197 0.00142

100 ->222 -0.00167

102 ->207 -0.00144

102 ->389 -0.00107

103 ->226 0.00140

103 ->231 0.00176

107 ->168 0.00285

110 ->231 0.00112

113 ->224 -0.00148

113 ->228 0.00160

113 ->234 -0.00109

114 ->229 0.00148

114 ->235 -0.00111

114 ->237 0.00103

115 ->168 0.00705

115 ->204 0.00103

119 ->197 0.00108

120 ->226 -0.00101

120 ->231 -0.00112

120 ->240 0.00156

120 ->244 -0.00108

120 ->276 -0.00141

121 ->168 -0.00104

121 ->229 0.00319

121 ->235 -0.00201

121 ->237 0.00112

121 ->279 0.00118

121 ->333 -0.00108

121 ->389 0.00145

122 ->168 0.00802

122 ->176 0.00109

122 ->204 0.00114

123 ->195 -0.00110

123 ->249 -0.00106

124 ->178 0.00271

124 ->179 0.00268

124 ->180 -0.00108

124 ->210 0.00119

124 ->227 0.00195

125 ->169 0.00640

125 ->175 0.00247

125 ->189 0.00326

126 ->222 -0.00115

126 ->253 0.00107

127 ->240 0.00298

127 ->244 -0.00232

127 ->254 0.00107

127 ->285 0.00105

127 ->343 -0.00126

128 ->168 0.01367

128 ->176 0.00102

128 ->183 0.00371

128 ->316 0.00106

129 ->228 -0.00155

129 ->234 0.00137

129 ->238 0.00103

130 ->168 0.00244

130 ->223 0.00148

130 ->229 0.00206

130 ->235 -0.00166

130 ->271 0.00185

130 ->279 0.00220

130 ->325 0.00146

130 ->333 -0.00118

131 ->228 0.00120

131 ->262 -0.00119

132 ->169 -0.00113

132 ->226 -0.00330

132 ->231 -0.00140

132 ->276 -0.00149

132 ->293 -0.00119

132 ->343 -0.00167

132 ->362 -0.00143

132 ->390 0.00140

133 ->179 0.00105

133 ->180 0.00199

133 ->186 0.00151

133 ->194 0.00172

133 ->222 -0.00110

133 ->225 0.00131

133 ->253 0.00113

133 ->261 -0.00148

133 ->277 -0.00134

134 ->168 -0.00270

134 ->229 0.00117

134 ->279 0.00115

135 ->168 -0.00443

135 ->192 -0.00113

135 ->196 -0.00121

135 ->229 -0.00158

135 ->271 -0.00159

135 ->304 0.00178

136 ->180 0.00114

136 ->186 0.00131

136 ->194 0.00200

136 ->225 0.00130

137 ->169 0.00145

137 ->226 -0.00119

138 ->195 -0.00102

138 ->228 -0.00111

138 ->262 0.00116

140 ->167 0.00110

143 ->168 0.00183

146 ->167 0.00111

146 ->172 0.00108

146 ->228 -0.00125

146 ->234 0.00115

147 ->167 -0.00514

147 ->172 0.00163

147 ->184 -0.00380

147 ->203 0.00147

148 ->169 0.00109

148 ->226 -0.00356

148 ->240 0.00202

148 ->244 -0.00159

148 ->247 -0.00108

148 ->258 -0.00167

148 ->343 -0.00112

149 ->170 -0.00120

149 ->179 -0.00265

149 ->180 -0.00754

149 ->186 -0.00613

149 ->190 -0.00145

149 ->194 -0.00391

149 ->197 -0.00162

149 ->198 0.00179

149 ->213 -0.00169

149 ->222 -0.00132

149 ->225 -0.00381

149 ->236 -0.00225

149 ->250 0.00198

149 ->253 -0.00242

149 ->259 -0.00190

149 ->260 0.00120

149 ->366 0.00177

149 ->371 -0.00102

149 ->378 -0.00162

149 ->393 0.00114

149 ->476 -0.00112

150 ->169 -0.00559

150 ->175 -0.00506

150 ->200 0.00586

150 ->221 0.00249

151 ->178 0.00197

151 ->179 0.00231

151 ->205 -0.00103

152 ->168 -0.01431

152 ->171 0.00177

152 ->176 -0.00381

152 ->183 0.00824

152 ->188 0.00105

152 ->204 0.00146

152 ->207 -0.00123

152 ->220 0.00176

153 ->168 0.07801

153 ->171 -0.00103

153 ->176 0.00146

153 ->183 -0.00925

153 ->192 -0.00148

153 ->201 0.00119

153 ->212 -0.00103

153 ->217 0.00114

153 ->220 -0.00106

153 ->223 0.00315

153 ->229 0.00215

153 ->235 -0.00150

153 ->237 -0.00121

153 ->246 -0.00127

153 ->248 -0.00102

153 ->263 -0.00181

153 ->271 -0.00185

153 ->287 0.00112

153 ->304 0.00131

154 ->168 -0.06919

154 ->171 0.00208

154 ->176 -0.00289

154 ->183 0.00422

154 ->204 0.00358

154 ->207 -0.00141

154 ->212 0.00132

154 ->220 0.00170

155 ->167 0.01143

155 ->172 0.00104

155 ->177 -0.00156

155 ->184 0.00223

156 ->169 -0.00354

156 ->173 0.00153

156 ->175 0.00150

156 ->189 0.00327

156 ->200 -0.00337

157 ->174 -0.00309

157 ->178 0.00155

157 ->179 0.00304

157 ->210 0.00101

158 ->168 -0.06625

158 ->176 -0.00141

158 ->183 0.00815

158 ->188 0.00229

158 ->196 -0.00167

158 ->201 0.00149

158 ->204 0.00140

158 ->217 0.00198

158 ->223 0.00253

158 ->229 0.00226

158 ->235 -0.00209

158 ->237 -0.00157

158 ->246 -0.00147

158 ->248 -0.00226

158 ->256 0.00120

158 ->263 -0.00249

158 ->271 -0.00206

158 ->350 0.00110

159 ->167 -0.00596

159 ->172 0.00479

159 ->177 -0.00262

159 ->184 -0.00108

160 ->174 0.00103

160 ->178 -0.00121

160 ->197 -0.00107

160 ->205 -0.00265

160 ->210 -0.00123

160 ->216 -0.00147

160 ->227 -0.00158

161 ->169 -0.02702

161 ->173 -0.00284

161 ->175 0.00243

161 ->189 0.00500

161 ->193 0.00155

161 ->200 -0.00957

161 ->215 0.00231

161 ->221 -0.00350

162 ->170 0.00521

162 ->174 0.00450

162 ->178 0.00431

162 ->179 0.00204

162 ->205 0.00428

162 ->210 0.00304

162 ->216 0.00154

162 ->227 0.00379

163 ->169 0.03819

163 ->173 -0.00711

163 ->175 0.00435

163 ->185 -0.00262

163 ->189 -0.01319

163 ->193 -0.00209

163 ->200 0.00933

163 ->206 0.00210

163 ->215 -0.00198

163 ->221 0.00377

163 ->326 0.00105

164 ->168 0.68986

164 ->171 -0.00337

164 ->176 0.00698

164 ->183 -0.01242

164 ->196 0.00118

164 ->201 0.00229

164 ->204 -0.01084

164 ->207 0.00283

164 ->212 -0.00444

164 ->217 -0.00211

164 ->220 -0.00657

164 ->223 0.00102

164 ->248 0.00157

164 ->265 -0.00177

165 ->167 -0.01861

165 ->172 0.00782

165 ->177 -0.00221

165 ->184 -0.01315

165 ->191 0.00144

165 ->202 -0.00112

165 ->203 0.00447

165 ->208 -0.00110

165 ->211 0.00170

165 ->219 0.00311

166 ->168 0.05663

166 ->171 -0.00690

166 ->176 -0.02303

166 ->183 0.00791

166 ->204 -0.00401

88 <-240 0.00103

89 <-194 0.00108

93 <-195 -0.00119

97 <-229 0.00100

100 <-180 0.00129

100 <-222 -0.00105

103 <-231 0.00119

107 <-168 0.00109

113 <-228 0.00105

115 <-168 0.00267

120 <-240 0.00104

120 <-276 -0.00101

121 <-229 0.00207

121 <-235 -0.00131

121 <-389 0.00115

122 <-168 0.00289

124 <-178 0.00138

124 <-179 0.00163

124 <-227 0.00134

125 <-169 0.00249

125 <-175 0.00114

125 <-189 0.00244

127 <-240 0.00193

127 <-244 -0.00151

128 <-183 0.00327

130 <-229 0.00134

130 <-235 -0.00103

130 <-271 0.00120

130 <-279 0.00155

130 <-325 0.00109

132 <-226 -0.00200

132 <-276 -0.00107

132 <-343 -0.00125

132 <-362 -0.00106

132 <-390 0.00108

135 <-304 0.00122

147 <-167 -0.00110

147 <-184 -0.00217

148 <-226 -0.00192

148 <-240 0.00115

149 <-179 -0.00129

149 <-180 -0.00290

149 <-186 -0.00255

149 <-194 -0.00176

149 <-225 -0.00205

149 <-236 -0.00133

149 <-250 0.00119

149 <-253 -0.00147

149 <-259 -0.00120

149 <-366 0.00129

149 <-378 -0.00120

150 <-169 -0.00505

150 <-175 -0.00231

150 <-200 0.00261

150 <-221 0.00151

152 <-168 0.00394

152 <-183 0.00547

153 <-183 -0.00631

153 <-204 0.00110

153 <-223 0.00164

153 <-271 -0.00125

154 <-168 0.00422

154 <-204 0.00157

156 <-169 0.00183

156 <-175 0.00133

156 <-189 0.00186

157 <-179 0.00160

158 <-168 0.00115

158 <-183 0.00510

158 <-188 0.00113

158 <-223 0.00117

158 <-229 0.00129

158 <-235 -0.00109

158 <-248 -0.00116

158 <-263 -0.00155

158 <-271 -0.00114

160 <-174 0.00101

160 <-179 -0.00278

160 <-205 -0.00125

160 <-227 -0.00125

161 <-169 0.00580

161 <-175 0.00273

161 <-189 0.00342

161 <-200 -0.00244

161 <-221 -0.00140

162 <-179 0.00494

162 <-180 -0.00171

162 <-205 0.00224

162 <-210 0.00153

162 <-216 0.00113

162 <-227 0.00221

163 <-169 -0.00582

163 <-173 -0.00148

163 <-175 -0.00256

163 <-185 -0.00125

163 <-189 -0.00758

163 <-200 0.00166

163 <-206 0.00142

163 <-221 0.00121

164 <-168 -0.01331

164 <-171 -0.00204

164 <-176 -0.00154

164 <-183 -0.00325

164 <-204 -0.00403

164 <-207 0.00116

164 <-212 -0.00142

164 <-217 -0.00126

164 <-220 -0.00290

165 <-167 0.00460

165 <-184 -0.00579

165 <-203 0.00187

165 <-219 0.00130

166 <-168 -0.01384

166 <-176 -0.00153

166 <-183 0.00351

166 <-204 -0.00139

Excited State 8: Singlet-E 3.6414 eV 340.48 nm f=0.0464 <S\*\*2>=0.000

51 ->230 0.00102

52 ->224 -0.00126

61 ->208 0.00116

61 ->238 -0.00114

62 ->206 0.00121

63 ->180 0.00127

75 ->240 -0.00103

84 ->182 0.00111

84 ->192 0.00112

84 ->196 0.00146

84 ->223 -0.00143

84 ->229 0.00101

85 ->278 -0.00112

88 ->190 -0.00108

88 ->194 -0.00170

88 ->197 -0.00133

88 ->222 -0.00110

88 ->230 -0.00102

89 ->206 0.00116

89 ->240 0.00146

89 ->244 -0.00121

93 ->182 -0.00134

93 ->192 -0.00112

93 ->196 -0.00193

93 ->223 0.00105

93 ->235 -0.00105

93 ->269 -0.00135

95 ->180 -0.00127

95 ->194 -0.00120

96 ->226 0.00133

97 ->208 0.00114

97 ->228 -0.00147

99 ->179 -0.00106

99 ->180 -0.00231

99 ->186 -0.00172

99 ->190 0.00104

99 ->197 0.00142

99 ->222 0.00167

100 ->206 0.00110

100 ->209 -0.00145

100 ->215 -0.00102

100 ->390 -0.00102

100 ->401 -0.00106

102 ->208 -0.00144

102 ->388 -0.00107

104 ->226 -0.00140

104 ->231 -0.00176

107 ->167 -0.00285

111 ->231 -0.00112

113 ->223 -0.00148

113 ->229 0.00160

113 ->235 -0.00109

114 ->228 -0.00148

114 ->234 0.00111

114 ->238 -0.00103

115 ->167 -0.00705

115 ->203 0.00103

119 ->226 0.00101

119 ->231 0.00112

119 ->240 0.00156

119 ->244 -0.00108

119 ->276 -0.00141

120 ->197 0.00108

121 ->167 -0.00104

121 ->228 -0.00319

121 ->234 0.00201

121 ->238 -0.00112

121 ->278 -0.00118

121 ->334 0.00108

121 ->388 -0.00145

122 ->167 -0.00802

122 ->177 0.00109

122 ->203 0.00114

123 ->196 0.00110

123 ->248 0.00106

124 ->169 -0.00640

124 ->175 -0.00247

124 ->189 0.00326

125 ->178 -0.00271

125 ->179 0.00268

125 ->180 -0.00108

125 ->210 -0.00119

125 ->227 -0.00195

126 ->240 0.00298

126 ->244 -0.00232

126 ->254 0.00107

126 ->285 0.00105

126 ->343 0.00126

127 ->222 0.00115

127 ->253 -0.00107

128 ->167 0.01367

128 ->177 -0.00102

128 ->184 0.00371

128 ->315 -0.00106

129 ->229 0.00155

129 ->235 -0.00137

129 ->237 -0.00103

130 ->167 -0.00244

130 ->224 0.00148

130 ->228 0.00206

130 ->234 -0.00166

130 ->272 -0.00185

130 ->278 0.00220

130 ->324 0.00146

130 ->334 -0.00118

131 ->229 0.00120

131 ->263 -0.00119

132 ->179 -0.00105

132 ->180 -0.00199

132 ->186 -0.00151

132 ->194 -0.00172

132 ->222 0.00110

132 ->225 -0.00131

132 ->253 -0.00113

132 ->261 -0.00148

132 ->277 0.00134

133 ->169 -0.00113

133 ->226 0.00330

133 ->231 0.00140

133 ->276 -0.00149

133 ->293 -0.00119

133 ->343 0.00167

133 ->362 0.00143

133 ->390 0.00140

134 ->167 0.00270

134 ->228 0.00117

134 ->278 0.00115

135 ->167 -0.00443

135 ->191 0.00113

135 ->195 0.00121

135 ->228 0.00158

135 ->272 -0.00159

135 ->305 0.00178

136 ->169 0.00145

136 ->226 0.00119

137 ->180 -0.00114

137 ->186 -0.00131

137 ->194 -0.00200

137 ->225 -0.00130

138 ->196 -0.00102

138 ->229 -0.00111

138 ->263 0.00116

140 ->168 -0.00110

143 ->167 -0.00183

146 ->168 0.00111

146 ->171 -0.00108

146 ->229 0.00125

146 ->235 -0.00115

147 ->168 0.00514

147 ->171 0.00163

147 ->183 0.00380

147 ->204 0.00147

148 ->170 -0.00120

148 ->179 0.00265

148 ->180 0.00754

148 ->186 0.00613

148 ->190 -0.00145

148 ->194 0.00391

148 ->197 -0.00162

148 ->198 -0.00179

148 ->213 0.00169

148 ->222 0.00132

148 ->225 0.00381

148 ->236 -0.00225

148 ->250 -0.00198

148 ->253 0.00242

148 ->259 -0.00190

148 ->260 -0.00120

148 ->366 -0.00177

148 ->371 -0.00102

148 ->378 0.00162

148 ->393 -0.00114

148 ->476 -0.00112

149 ->169 0.00109

149 ->226 0.00356

149 ->240 0.00202

149 ->244 -0.00159

149 ->247 0.00108

149 ->258 0.00167

149 ->343 0.00112

150 ->178 0.00197

150 ->179 -0.00231

150 ->205 -0.00103

151 ->169 -0.00559

151 ->175 -0.00506

151 ->200 0.00586

151 ->221 0.00249

152 ->167 0.01431

152 ->172 0.00177

152 ->177 -0.00381

152 ->184 -0.00824

152 ->187 0.00105

152 ->203 0.00146

152 ->208 -0.00123

152 ->219 0.00176

153 ->167 -0.07801

153 ->172 -0.00103

153 ->177 0.00146

153 ->184 0.00925

153 ->191 -0.00148

153 ->202 0.00119

153 ->211 -0.00103

153 ->218 0.00114

153 ->219 -0.00106

153 ->224 0.00315

153 ->228 0.00215

153 ->234 -0.00150

153 ->238 -0.00121

153 ->245 -0.00127

153 ->249 -0.00102

153 ->262 -0.00181

153 ->272 0.00185

153 ->288 0.00112

153 ->305 -0.00131

154 ->167 -0.06919

154 ->172 -0.00208

154 ->177 0.00289

154 ->184 0.00422

154 ->203 -0.00358

154 ->208 0.00141

154 ->211 -0.00132

154 ->219 -0.00170

155 ->168 0.01143

155 ->171 -0.00104

155 ->176 0.00156

155 ->183 0.00223

156 ->174 0.00309

156 ->178 0.00155

156 ->179 -0.00304

156 ->210 0.00101

157 ->169 -0.00354

157 ->173 -0.00153

157 ->175 0.00150

157 ->189 -0.00327

157 ->200 -0.00337

158 ->167 0.06625

158 ->177 -0.00141

158 ->184 -0.00815

158 ->187 0.00229

158 ->195 -0.00167

158 ->202 0.00149

158 ->203 0.00140

158 ->218 0.00198

158 ->224 0.00253

158 ->228 0.00226

158 ->234 -0.00209

158 ->238 -0.00157

158 ->245 -0.00147

158 ->249 -0.00226

158 ->257 0.00120

158 ->262 -0.00249

158 ->272 0.00206

158 ->349 0.00110

159 ->168 0.00596

159 ->171 0.00479

159 ->176 -0.00262

159 ->183 0.00108

160 ->169 0.02702

160 ->173 -0.00284

160 ->175 -0.00243

160 ->189 0.00500

160 ->193 -0.00155

160 ->200 0.00957

160 ->215 -0.00231

160 ->221 0.00350

161 ->174 0.00103

161 ->178 0.00121

161 ->197 0.00107

161 ->205 0.00265

161 ->210 0.00123

161 ->216 0.00147

161 ->227 0.00158

162 ->169 -0.03819

162 ->173 -0.00711

162 ->175 -0.00435

162 ->185 -0.00262

162 ->189 -0.01319

162 ->193 0.00209

162 ->200 -0.00933

162 ->206 0.00210

162 ->215 0.00198

162 ->221 -0.00377

162 ->326 -0.00105

163 ->170 -0.00521

163 ->174 0.00450

163 ->178 -0.00431

163 ->179 0.00204

163 ->205 -0.00428

163 ->210 -0.00304

163 ->216 -0.00154

163 ->227 -0.00379

164 ->167 0.68986

164 ->172 0.00337

164 ->177 -0.00698

164 ->184 -0.01242

164 ->195 -0.00118

164 ->202 -0.00229

164 ->203 0.01084

164 ->208 -0.00283

164 ->211 0.00444

164 ->218 0.00211

164 ->219 0.00657

164 ->224 -0.00102

164 ->249 -0.00157

164 ->266 0.00177

165 ->168 -0.01861

165 ->171 -0.00782

165 ->176 0.00221

165 ->183 -0.01315

165 ->192 -0.00144

165 ->201 0.00112

165 ->204 -0.00447

165 ->207 0.00110

165 ->212 -0.00170

165 ->220 -0.00311

166 ->167 -0.05663

166 ->172 -0.00690

166 ->177 -0.02303

166 ->184 -0.00791

166 ->203 -0.00401

88 <-194 -0.00108

89 <-240 0.00103

93 <-196 -0.00119

97 <-228 -0.00100

99 <-180 -0.00129

99 <-222 0.00105

104 <-231 -0.00119

107 <-167 -0.00109

113 <-229 0.00105

115 <-167 -0.00267

119 <-240 0.00104

119 <-276 -0.00101

121 <-228 -0.00207

121 <-234 0.00131

121 <-388 -0.00115

122 <-167 -0.00289

124 <-169 -0.00249

124 <-175 -0.00114

124 <-189 0.00244

125 <-178 -0.00138

125 <-179 0.00163

125 <-227 -0.00134

126 <-240 0.00193

126 <-244 -0.00151

128 <-184 0.00327

130 <-228 0.00134

130 <-234 -0.00103

130 <-272 -0.00120

130 <-278 0.00155

130 <-324 0.00109

133 <-226 0.00200

133 <-276 -0.00107

133 <-343 0.00125

133 <-362 0.00106

133 <-390 0.00108

135 <-305 0.00122

147 <-168 0.00110

147 <-183 0.00217

148 <-179 0.00129

148 <-180 0.00290

148 <-186 0.00255

148 <-194 0.00176

148 <-225 0.00205

148 <-236 -0.00133

148 <-250 -0.00119

148 <-253 0.00147

148 <-259 -0.00120

148 <-366 -0.00129

148 <-378 0.00120

149 <-226 0.00192

149 <-240 0.00115

151 <-169 -0.00505

151 <-175 -0.00231

151 <-200 0.00261

151 <-221 0.00151

152 <-167 -0.00394

152 <-184 -0.00547

153 <-184 0.00631

153 <-203 0.00110

153 <-224 0.00164

153 <-272 0.00125

154 <-167 0.00422

154 <-203 -0.00157

156 <-179 -0.00160

157 <-169 0.00183

157 <-175 0.00133

157 <-189 -0.00186

158 <-167 -0.00115

158 <-184 -0.00510

158 <-187 0.00113

158 <-224 0.00117

158 <-228 0.00129

158 <-234 -0.00109

158 <-249 -0.00116

158 <-262 -0.00155

158 <-272 0.00114

160 <-169 -0.00580

160 <-175 -0.00273

160 <-189 0.00342

160 <-200 0.00244

160 <-221 0.00140

161 <-174 0.00101

161 <-179 -0.00278

161 <-205 0.00125

161 <-227 0.00125

162 <-169 0.00582

162 <-173 -0.00148

162 <-175 0.00256

162 <-185 -0.00125

162 <-189 -0.00758

162 <-200 -0.00166

162 <-206 0.00142

162 <-221 -0.00121

163 <-179 0.00494

163 <-180 -0.00171

163 <-205 -0.00224

163 <-210 -0.00153

163 <-216 -0.00113

163 <-227 -0.00221

164 <-167 -0.01331

164 <-172 0.00204

164 <-177 0.00154

164 <-184 -0.00325

164 <-203 0.00403

164 <-208 -0.00116

164 <-211 0.00142

164 <-218 0.00126

164 <-219 0.00290

165 <-168 0.00460

165 <-183 -0.00579

165 <-204 -0.00187

165 <-220 -0.00130

166 <-167 0.01384

166 <-177 -0.00153

166 <-184 -0.00351

166 <-203 -0.00139

Excited State 9: Singlet-E 3.7142 eV 333.81 nm f=0.0233 <S\*\*2>=0.000

50 ->179 -0.00125

52 ->168 0.00139

62 ->179 0.00121

93 ->203 0.00111

95 ->189 0.00151

97 ->183 0.00182

98 ->183 0.00100

99 ->169 0.00165

99 ->189 0.00163

102 ->168 -0.00167

102 ->183 0.00225

113 ->167 -0.00112

124 ->180 -0.00107

124 ->225 -0.00143

127 ->169 -0.00111

128 ->168 -0.00193

130 ->168 -0.00195

130 ->183 0.00178

131 ->167 0.00203

131 ->184 0.00122

132 ->169 0.00253

134 ->168 0.00222

135 ->168 -0.00531

135 ->183 -0.00589

135 ->201 -0.00107

135 ->204 0.00405

135 ->220 0.00155

135 ->397 0.00128

136 ->179 0.00108

138 ->167 -0.00238

138 ->184 -0.00101

139 ->183 0.00130

140 ->167 -0.00144

141 ->169 0.00243

144 ->169 0.00232

145 ->179 -0.00132

147 ->167 0.00118

148 ->169 0.03423

148 ->175 0.00758

148 ->189 0.00137

148 ->193 -0.00209

148 ->200 0.00597

148 ->215 -0.00119

148 ->221 0.00185

148 ->254 -0.00115

149 ->170 -0.00150

149 ->174 0.00312

149 ->178 -0.00324

149 ->179 -0.01731

149 ->180 0.00636

149 ->194 0.00101

149 ->210 -0.00204

149 ->227 -0.00355

151 ->180 -0.00112

152 ->168 0.01228

152 ->183 -0.00112

153 ->168 0.38270

153 ->171 0.00605

153 ->176 0.01199

153 ->183 -0.00975

153 ->204 0.00133

153 ->248 0.00109

154 ->176 0.00130

155 ->167 0.00562

155 ->172 -0.00139

157 ->170 0.00149

158 ->168 0.59108

158 ->171 0.00547

158 ->176 0.01527

158 ->182 -0.00112

158 ->183 -0.01340

158 ->212 -0.00159

158 ->223 0.00102

158 ->248 0.00171

158 ->339 -0.00103

159 ->167 0.00121

159 ->172 -0.00102

160 ->170 -0.00123

161 ->169 0.00206

161 ->175 -0.00142

162 ->178 -0.00154

162 ->180 -0.00360

162 ->186 -0.00239

162 ->198 0.00121

162 ->205 0.00137

162 ->225 -0.00188

162 ->239 0.00102

163 ->169 0.00424

163 ->175 0.00158

163 ->189 0.00165

163 ->200 -0.00101

164 ->168 0.01630

164 ->183 0.00283

164 ->223 0.00141

165 ->167 0.02168

165 ->172 0.00212

165 ->177 0.00265

166 ->168 -0.02393

166 ->176 0.00532

166 ->183 -0.00211

166 ->204 -0.00119

166 ->223 0.00181

135 <-183 0.00116

149 <-179 0.00274

149 <-205 0.00152

152 <-168 -0.00168

153 <-168 -0.00189

153 <-183 0.00135

158 <-168 -0.00351

158 <-183 0.00106

158 <-204 -0.00161

162 <-179 0.00133

164 <-183 0.00126

165 <-167 -0.00580

165 <-228 0.00163

165 <-272 0.00149

166 <-168 0.00490

166 <-229 -0.00168

166 <-271 0.00138

Excited State 10: Singlet-E 3.7142 eV 333.81 nm f=0.0233 <S\*\*2>=0.000

51 ->179 -0.00125

52 ->167 0.00139

63 ->179 0.00121

93 ->204 -0.00111

96 ->189 0.00151

97 ->184 -0.00182

98 ->184 -0.00100

100 ->169 -0.00165

100 ->189 0.00163

102 ->167 -0.00167

102 ->184 0.00225

113 ->168 -0.00112

125 ->180 0.00107

125 ->225 0.00143

126 ->169 0.00111

128 ->167 0.00193

130 ->167 -0.00195

130 ->184 0.00178

131 ->168 0.00203

131 ->183 0.00122

133 ->169 -0.00253

134 ->167 0.00222

135 ->167 0.00531

135 ->184 0.00589

135 ->202 -0.00107

135 ->203 0.00405

135 ->219 0.00155

135 ->398 0.00128

137 ->179 0.00108

138 ->168 -0.00238

138 ->183 -0.00101

139 ->184 -0.00130

140 ->168 -0.00144

142 ->169 -0.00243

144 ->179 -0.00132

145 ->169 -0.00232

147 ->168 0.00118

148 ->170 0.00150

148 ->174 0.00312

148 ->178 0.00324

148 ->179 -0.01731

148 ->180 0.00636

148 ->194 0.00101

148 ->210 0.00204

148 ->227 0.00355

149 ->169 -0.03423

149 ->175 -0.00758

149 ->189 0.00137

149 ->193 0.00209

149 ->200 -0.00597

149 ->215 0.00119

149 ->221 -0.00185

149 ->254 0.00115

150 ->180 -0.00112

152 ->167 0.01228

152 ->184 -0.00112

153 ->167 0.38270

153 ->172 -0.00605

153 ->177 -0.01199

153 ->184 -0.00975

153 ->203 -0.00133

153 ->249 -0.00109

154 ->177 0.00130

155 ->168 -0.00562

155 ->171 -0.00139

156 ->170 -0.00149

158 ->167 0.59108

158 ->172 -0.00547

158 ->177 -0.01527

158 ->181 0.00112

158 ->184 -0.01340

158 ->211 0.00159

158 ->224 -0.00102

158 ->249 -0.00171

158 ->338 -0.00103

159 ->168 0.00121

159 ->171 0.00102

160 ->169 0.00206

160 ->175 -0.00142

161 ->170 -0.00123

162 ->169 0.00424

162 ->175 0.00158

162 ->189 -0.00165

162 ->200 -0.00101

163 ->178 -0.00154

163 ->180 0.00360

163 ->186 0.00239

163 ->198 -0.00121

163 ->205 0.00137

163 ->225 0.00188

163 ->239 -0.00102

164 ->167 -0.01630

164 ->184 -0.00283

164 ->224 0.00141

165 ->168 -0.02168

165 ->171 0.00212

165 ->176 0.00265

166 ->167 -0.02393

166 ->177 -0.00532

166 ->184 -0.00211

166 ->203 0.00119

166 ->224 -0.00181

135 <-184 -0.00116

148 <-179 0.00274

148 <-205 -0.00152

152 <-167 -0.00168

153 <-167 -0.00189

153 <-184 0.00135

158 <-167 -0.00351

158 <-184 0.00106

158 <-203 0.00161

163 <-179 -0.00133

164 <-184 -0.00126

165 <-168 0.00580

165 <-229 0.00163

165 <-271 -0.00149

166 <-167 0.00490

166 <-228 0.00168

166 <-272 0.00138

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

Leave Link 914 at Thu Sep 5 22:07:15 2019, MaxMem= 1342177280 cpu: 14234.8

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

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

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Population analysis using the SCF density.

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Orbital symmetries:

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

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

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

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

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

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

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

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

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

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -14.30274 -14.30274 -14.30273 -14.30273 -10.20850

Alpha occ. eigenvalues -- -10.20850 -10.20850 -10.20850 -10.20849 -10.20849

Alpha occ. eigenvalues -- -10.20849 -10.20849 -10.19527 -10.19527 -10.19527

Alpha occ. eigenvalues -- -10.19527 -10.18649 -10.18649 -10.18649 -10.18649

Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17325 -10.17325

Alpha occ. eigenvalues -- -10.17325 -10.17325 -10.17325 -10.17283 -10.17283

Alpha occ. eigenvalues -- -10.17283 -10.17283 -10.17252 -10.17252 -10.17252

Alpha occ. eigenvalues -- -10.17252 -10.17215 -10.17215 -10.17215 -10.17215

Alpha occ. eigenvalues -- -10.16829 -10.16829 -10.16829 -10.16829 -10.16763

Alpha occ. eigenvalues -- -10.16763 -10.16763 -10.16763 -0.96311 -0.95466

Alpha occ. eigenvalues -- -0.95466 -0.94579 -0.86920 -0.86555 -0.86555

Alpha occ. eigenvalues -- -0.86379 -0.82290 -0.80635 -0.80635 -0.78864

Alpha occ. eigenvalues -- -0.76631 -0.76592 -0.76592 -0.76144 -0.74941

Alpha occ. eigenvalues -- -0.74862 -0.74862 -0.74828 -0.74123 -0.73406

Alpha occ. eigenvalues -- -0.73406 -0.71852 -0.70867 -0.66163 -0.66163

Alpha occ. eigenvalues -- -0.62134 -0.61068 -0.60823 -0.60823 -0.60677

Alpha occ. eigenvalues -- -0.59897 -0.59897 -0.59468 -0.59445 -0.58587

Alpha occ. eigenvalues -- -0.57012 -0.56547 -0.56261 -0.56261 -0.56057

Alpha occ. eigenvalues -- -0.55332 -0.55332 -0.54829 -0.54320 -0.52699

Alpha occ. eigenvalues -- -0.52699 -0.52628 -0.51909 -0.51398 -0.51398

Alpha occ. eigenvalues -- -0.49894 -0.49806 -0.49165 -0.49165 -0.46156

Alpha occ. eigenvalues -- -0.46073 -0.45862 -0.45731 -0.45731 -0.44985

Alpha occ. eigenvalues -- -0.44985 -0.44864 -0.44341 -0.42569 -0.42546

Alpha occ. eigenvalues -- -0.42305 -0.42305 -0.42195 -0.42155 -0.42155

Alpha occ. eigenvalues -- -0.42129 -0.41797 -0.41216 -0.40818 -0.40818

Alpha occ. eigenvalues -- -0.40139 -0.40139 -0.39299 -0.39066 -0.38439

Alpha occ. eigenvalues -- -0.38303 -0.37820 -0.37820 -0.36828 -0.36767

Alpha occ. eigenvalues -- -0.36708 -0.36708 -0.35813 -0.35163 -0.34764

Alpha occ. eigenvalues -- -0.34695 -0.34695 -0.34605 -0.34599 -0.34599

Alpha occ. eigenvalues -- -0.33902 -0.31870 -0.31301 -0.31301 -0.28611

Alpha occ. eigenvalues -- -0.28611 -0.26425 -0.26019 -0.25991 -0.25945

Alpha occ. eigenvalues -- -0.25930 -0.25930 -0.25682 -0.25255 -0.25238

Alpha occ. eigenvalues -- -0.25238 -0.24717 -0.24717 -0.24647 -0.20184

Alpha occ. eigenvalues -- -0.18937

Alpha virt. eigenvalues -- -0.09064 -0.09064 -0.03556 -0.01361 -0.01316

Alpha virt. eigenvalues -- -0.01316 -0.01116 -0.01041 -0.01029 -0.00930

Alpha virt. eigenvalues -- -0.00930 0.03358 0.03798 0.04518 0.04646

Alpha virt. eigenvalues -- 0.04646 0.05596 0.05596 0.05822 0.06119

Alpha virt. eigenvalues -- 0.07000 0.07000 0.07197 0.08446 0.08983

Alpha virt. eigenvalues -- 0.08983 0.09147 0.09179 0.09557 0.09557

Alpha virt. eigenvalues -- 0.10009 0.10277 0.10339 0.10376 0.11364

Alpha virt. eigenvalues -- 0.11364 0.11918 0.11918 0.12037 0.12647

Alpha virt. eigenvalues -- 0.13045 0.13045 0.13326 0.13423 0.13695

Alpha virt. eigenvalues -- 0.13695 0.13809 0.14078 0.14170 0.14728

Alpha virt. eigenvalues -- 0.15121 0.15121 0.15773 0.15773 0.16274

Alpha virt. eigenvalues -- 0.16461 0.18510 0.18510 0.20796 0.21632

Alpha virt. eigenvalues -- 0.22463 0.23766 0.23766 0.23814 0.23862

Alpha virt. eigenvalues -- 0.24494 0.25350 0.25688 0.25688 0.26612

Alpha virt. eigenvalues -- 0.26946 0.26946 0.27152 0.27581 0.28038

Alpha virt. eigenvalues -- 0.28054 0.28054 0.28372 0.28519 0.28519

Alpha virt. eigenvalues -- 0.28918 0.29009 0.29009 0.29010 0.29992

Alpha virt. eigenvalues -- 0.29992 0.30039 0.30049 0.30669 0.31413

Alpha virt. eigenvalues -- 0.31413 0.31596 0.32476 0.34392 0.35120

Alpha virt. eigenvalues -- 0.35359 0.35359 0.35508 0.36081 0.36081

Alpha virt. eigenvalues -- 0.36373 0.36473 0.36753 0.36753 0.36852

Alpha virt. eigenvalues -- 0.36852 0.37487 0.37665 0.38134 0.38779

Alpha virt. eigenvalues -- 0.38849 0.39795 0.39795 0.39797 0.39867

Alpha virt. eigenvalues -- 0.39867 0.40128 0.40540 0.40793 0.41155

Alpha virt. eigenvalues -- 0.41200 0.41200 0.41478 0.41535 0.41535

Alpha virt. eigenvalues -- 0.41912 0.41955 0.41990 0.41990 0.42349

Alpha virt. eigenvalues -- 0.42980 0.42980 0.43152 0.43431 0.43431

Alpha virt. eigenvalues -- 0.43723 0.43879 0.44575 0.44575 0.44601

Alpha virt. eigenvalues -- 0.44829 0.45046 0.45147 0.45219 0.45219

Alpha virt. eigenvalues -- 0.45518 0.46539 0.46539 0.46774 0.46774

Alpha virt. eigenvalues -- 0.46835 0.47207 0.47595 0.48416 0.48416

Alpha virt. eigenvalues -- 0.48766 0.48766 0.49664 0.49664 0.49995

Alpha virt. eigenvalues -- 0.49999 0.50136 0.51020 0.51114 0.51349

Alpha virt. eigenvalues -- 0.51782 0.52598 0.52598 0.53594 0.53594

Alpha virt. eigenvalues -- 0.53679 0.54246 0.54246 0.54286 0.54884

Alpha virt. eigenvalues -- 0.55960 0.56631 0.57532 0.57677 0.57677

Alpha virt. eigenvalues -- 0.57715 0.57900 0.58626 0.58626 0.59659

Alpha virt. eigenvalues -- 0.59659 0.60331 0.60460 0.60602 0.60839

Alpha virt. eigenvalues -- 0.60839 0.61152 0.61323 0.61323 0.61386

Alpha virt. eigenvalues -- 0.61510 0.61516 0.61657 0.61657 0.62106

Alpha virt. eigenvalues -- 0.62516 0.62617 0.62617 0.62762 0.63648

Alpha virt. eigenvalues -- 0.63898 0.63898 0.64424 0.64555 0.64836

Alpha virt. eigenvalues -- 0.64836 0.65153 0.65227 0.65335 0.65437

Alpha virt. eigenvalues -- 0.65437 0.65564 0.66823 0.66823 0.66881

Alpha virt. eigenvalues -- 0.67116 0.67968 0.67968 0.68150 0.69635

Alpha virt. eigenvalues -- 0.69635 0.70395 0.70711 0.72180 0.72180

Alpha virt. eigenvalues -- 0.72611 0.72611 0.72694 0.73045 0.73289

Alpha virt. eigenvalues -- 0.73760 0.73787 0.73787 0.74429 0.74493

Alpha virt. eigenvalues -- 0.75337 0.75337 0.75723 0.75848 0.75848

Alpha virt. eigenvalues -- 0.75952 0.76469 0.76469 0.77006 0.78250

Alpha virt. eigenvalues -- 0.78260 0.78869 0.78869 0.79700 0.79743

Alpha virt. eigenvalues -- 0.79990 0.80537 0.80537 0.81093 0.81093

Alpha virt. eigenvalues -- 0.81419 0.81953 0.82369 0.82664 0.82664

Alpha virt. eigenvalues -- 0.84132 0.84615 0.85250 0.85250 0.85690

Alpha virt. eigenvalues -- 0.85794 0.87013 0.87285 0.87285 0.87398

Alpha virt. eigenvalues -- 0.89301 0.89301 0.89302 0.89497 0.90001

Alpha virt. eigenvalues -- 0.90001 0.90117 0.91772 0.92560 0.92684

Alpha virt. eigenvalues -- 0.92684 0.93361 0.93558 0.94473 0.94473

Alpha virt. eigenvalues -- 0.94991 0.96109 0.96620 0.96788 0.96788

Alpha virt. eigenvalues -- 0.98372 0.99146 0.99146 1.00407 1.00505

Alpha virt. eigenvalues -- 1.01503 1.01503 1.02404 1.02469 1.02827

Alpha virt. eigenvalues -- 1.04412 1.04412 1.05228 1.05228 1.05341

Alpha virt. eigenvalues -- 1.05453 1.05932 1.07581 1.08591 1.09226

Alpha virt. eigenvalues -- 1.09226 1.09719 1.11356 1.11356 1.11644

Alpha virt. eigenvalues -- 1.12557 1.13167 1.13167 1.14992 1.14992

Alpha virt. eigenvalues -- 1.15230 1.15462 1.15462 1.16885 1.17514

Alpha virt. eigenvalues -- 1.17514 1.17633 1.17633 1.17867 1.18328

Alpha virt. eigenvalues -- 1.19469 1.20497 1.20497 1.20958 1.21019

Alpha virt. eigenvalues -- 1.21094 1.21438 1.21438 1.21749 1.21749

Alpha virt. eigenvalues -- 1.22277 1.22828 1.22971 1.23975 1.24161

Alpha virt. eigenvalues -- 1.24161 1.24766 1.24766 1.25277 1.25326

Alpha virt. eigenvalues -- 1.25676 1.26445 1.27012 1.27012 1.27775

Alpha virt. eigenvalues -- 1.28531 1.28531 1.28827 1.30246 1.31486

Alpha virt. eigenvalues -- 1.31806 1.32636 1.32636 1.37143 1.38170

Alpha virt. eigenvalues -- 1.38595 1.38595 1.40391 1.40391 1.41032

Alpha virt. eigenvalues -- 1.41255 1.41741 1.43969 1.43969 1.44475

Alpha virt. eigenvalues -- 1.45941 1.47242 1.47242 1.47706 1.47723

Alpha virt. eigenvalues -- 1.48059 1.48534 1.48534 1.48539 1.49294

Alpha virt. eigenvalues -- 1.49994 1.49994 1.50305 1.50690 1.52899

Alpha virt. eigenvalues -- 1.52899 1.53718 1.54174 1.54451 1.54451

Alpha virt. eigenvalues -- 1.55548 1.55548 1.55715 1.56727 1.56727

Alpha virt. eigenvalues -- 1.57149 1.58563 1.59949 1.61260 1.61260

Alpha virt. eigenvalues -- 1.61460 1.61682 1.62535 1.62535 1.64836

Alpha virt. eigenvalues -- 1.64836 1.65259 1.67334 1.68458 1.68666

Alpha virt. eigenvalues -- 1.68666 1.68773 1.70139 1.70207 1.70207

Alpha virt. eigenvalues -- 1.71110 1.71110 1.71694 1.73965 1.74279

Alpha virt. eigenvalues -- 1.74716 1.76064 1.76064 1.76158 1.76287

Alpha virt. eigenvalues -- 1.76357 1.76357 1.77480 1.77480 1.77707

Alpha virt. eigenvalues -- 1.79010 1.79082 1.79905 1.80586 1.80586

Alpha virt. eigenvalues -- 1.81095 1.81289 1.81399 1.81830 1.81830

Alpha virt. eigenvalues -- 1.83685 1.83685 1.84124 1.84128 1.84558

Alpha virt. eigenvalues -- 1.84787 1.85072 1.85222 1.85222 1.86524

Alpha virt. eigenvalues -- 1.87566 1.87566 1.88657 1.88870 1.88870

Alpha virt. eigenvalues -- 1.89088 1.89660 1.89981 1.91737 1.91971

Alpha virt. eigenvalues -- 1.91971 1.92211 1.92565 1.92713 1.92785

Alpha virt. eigenvalues -- 1.92785 1.93158 1.93232 1.93232 1.94017

Alpha virt. eigenvalues -- 1.94080 1.94121 1.94121 1.94591 1.96178

Alpha virt. eigenvalues -- 1.96407 1.96407 1.96689 1.96971 1.96971

Alpha virt. eigenvalues -- 1.98495 1.99902 1.99997 1.99997 2.00083

Alpha virt. eigenvalues -- 2.00213 2.00556 2.00556 2.01260 2.06900

Alpha virt. eigenvalues -- 2.07144 2.08170 2.08170 2.09100 2.09100

Alpha virt. eigenvalues -- 2.09104 2.11700 2.13063 2.13904 2.14304

Alpha virt. eigenvalues -- 2.14304 2.19160 2.22089 2.23720 2.24110

Alpha virt. eigenvalues -- 2.24110 2.25803 2.25876 2.25876 2.26301

Alpha virt. eigenvalues -- 2.26583 2.26836 2.27625 2.27625 2.27835

Alpha virt. eigenvalues -- 2.28125 2.28341 2.28341 2.28682 2.29592

Alpha virt. eigenvalues -- 2.29592 2.29659 2.29877 2.30520 2.30520

Alpha virt. eigenvalues -- 2.32006 2.32115 2.32445 2.33142 2.33142

Alpha virt. eigenvalues -- 2.33973 2.33973 2.35654 2.35762 2.36440

Alpha virt. eigenvalues -- 2.36729 2.36729 2.36832 2.38526 2.38738

Alpha virt. eigenvalues -- 2.39662 2.39662 2.40442 2.40442 2.40919

Alpha virt. eigenvalues -- 2.44253 2.44865 2.44865 2.44970 2.47256

Alpha virt. eigenvalues -- 2.47341 2.49851 2.49851 2.53871 2.54681

Alpha virt. eigenvalues -- 2.54681 2.54903 2.55451 2.57018 2.57718

Alpha virt. eigenvalues -- 2.57972 2.57972 2.59297 2.59374 2.59374

Alpha virt. eigenvalues -- 2.60402 2.61072 2.61072 2.62117 2.62454

Alpha virt. eigenvalues -- 2.62674 2.62770 2.64559 2.64559 2.65206

Alpha virt. eigenvalues -- 2.65206 2.65617 2.65620 2.68503 2.69773

Alpha virt. eigenvalues -- 2.70071 2.70071 2.70289 2.72767 2.72767

Alpha virt. eigenvalues -- 2.73257 2.74889 2.74889 2.75016 2.75043

Alpha virt. eigenvalues -- 2.77012 2.77012 2.78467 2.78610 2.79432

Alpha virt. eigenvalues -- 2.79445 2.79445 2.80399 2.80679 2.82656

Alpha virt. eigenvalues -- 2.82656 2.84183 2.84843 2.85481 2.85481

Alpha virt. eigenvalues -- 2.85969 2.87050 2.89784 2.89784 2.90174

Alpha virt. eigenvalues -- 2.90174 2.90673 2.92973 2.94116 2.95892

Alpha virt. eigenvalues -- 2.95892 2.96850 2.98852 2.98852 2.99046

Alpha virt. eigenvalues -- 2.99721 3.01290 3.02782 3.04316 3.04877

Alpha virt. eigenvalues -- 3.04877 3.06540 3.07481 3.07481 3.07582

Alpha virt. eigenvalues -- 3.08395 3.08395 3.09189 3.11350 3.11687

Alpha virt. eigenvalues -- 3.11860 3.12217 3.12217 3.14525 3.16838

Alpha virt. eigenvalues -- 3.16838 3.16849 3.19546 3.19619 3.19619

Alpha virt. eigenvalues -- 3.19736 3.22486 3.25834 3.25947 3.25947

Alpha virt. eigenvalues -- 3.26087 3.26816 3.26816 3.29255 3.29591

Alpha virt. eigenvalues -- 3.29591 3.29856 3.29976 3.29996 3.30214

Alpha virt. eigenvalues -- 3.30214 3.30436 3.31091 3.31193 3.31272

Alpha virt. eigenvalues -- 3.31272 3.31847 3.32135 3.34686 3.34686

Alpha virt. eigenvalues -- 3.34715 3.35837 3.35837 3.36785 3.38248

Alpha virt. eigenvalues -- 3.38248 3.39729 3.40864 3.42407 3.43091

Alpha virt. eigenvalues -- 3.43091 3.44709 3.50363 3.51898 3.51956

Alpha virt. eigenvalues -- 3.51956 3.56786 3.58143 3.58143 3.58602

Alpha virt. eigenvalues -- 3.58602 3.59419 3.59738 3.61534 3.62677

Alpha virt. eigenvalues -- 3.66704 3.67307 3.67307 3.72803 3.73568

Alpha virt. eigenvalues -- 3.75789 3.75789 3.82769 3.82769 3.82872

Alpha virt. eigenvalues -- 3.85007 3.87457 3.87457 3.89144 3.91617

Alpha virt. eigenvalues -- 3.93980 3.93980 3.95111 3.95447 3.96267

Alpha virt. eigenvalues -- 3.96313 3.96313 3.96391 3.99534 4.01085

Alpha virt. eigenvalues -- 4.01085 4.12026 4.33381 4.35441 4.40179

Alpha virt. eigenvalues -- 4.40179 4.46726 4.49709 4.54091 4.54091

Alpha virt. eigenvalues -- 4.61897 4.66888 4.66888 4.67840 4.78821

Alpha virt. eigenvalues -- 4.78831 4.78831 4.78841 5.11536 5.18916

Alpha virt. eigenvalues -- 5.18916 5.32589 7.77675 7.77675 7.88025

Alpha virt. eigenvalues -- 7.92778 8.13982 11.12048 23.25291 23.28974

Alpha virt. eigenvalues -- 23.28974 23.30653 23.46369 23.53063 23.53063

Alpha virt. eigenvalues -- 23.57714 23.74795 23.75935 23.75935 23.77727

Alpha virt. eigenvalues -- 23.81067 23.81232 23.81232 23.81492 23.85161

Alpha virt. eigenvalues -- 23.86126 23.86126 23.86887 23.92662 23.94755

Alpha virt. eigenvalues -- 23.94755 23.96993 23.98200 23.99159 23.99159

Alpha virt. eigenvalues -- 23.99221 24.04793 24.04950 24.04950 24.05134

Alpha virt. eigenvalues -- 24.08773 24.09280 24.09280 24.09729 24.13357

Alpha virt. eigenvalues -- 24.13718 24.13718 24.14422 24.16343 24.16382

Alpha virt. eigenvalues -- 24.16382 24.16394 35.63343 35.64463 35.66095

Alpha virt. eigenvalues -- 35.66095

Condensed to atoms (all electrons):

Mulliken charges:

1

1 C -0.261143

2 C 0.308669

3 N -0.706255

4 C 0.308669

5 C -0.261143

6 C -0.149008

7 C 0.308669

8 N -0.706255

9 C 0.308669

10 C -0.261143

11 C -0.261143

12 C -0.149008

13 C 0.308669

14 C -0.261143

15 C -0.261143

16 C 0.308669

17 N -0.706255

18 C -0.149008

19 C 0.308669

20 C -0.261143

21 C -0.261143

22 C 0.308669

23 N -0.706255

24 C -0.149008

25 C -0.105849

26 C -0.211897

27 C -0.217879

28 C -0.221701

29 C -0.217879

30 C -0.211897

31 C -0.221701

32 C -0.217879

33 C -0.211897

34 C -0.105849

35 C -0.211897

36 C -0.217879

37 C -0.105849

38 C -0.211897

39 C -0.217879

40 C -0.221701

41 C -0.217879

42 C -0.211897

43 C -0.105849

44 C -0.211897

45 C -0.217879

46 C -0.221701

47 C -0.217879

48 C -0.211897

49 H 0.239146

50 H 0.239146

51 H 0.239146

52 H 0.239146

53 H 0.239146

54 H 0.239146

55 H 0.239146

56 H 0.239146

57 H 0.224238

58 H 0.225860

59 H 0.225719

60 H 0.225860

61 H 0.224238

62 H 0.225719

63 H 0.225860

64 H 0.224238

65 H 0.224238

66 H 0.225860

67 H 0.224238

68 H 0.225860

69 H 0.225719

70 H 0.225860

71 H 0.224238

72 H 0.224238

73 H 0.225860

74 H 0.225719

75 H 0.225860

76 H 0.224238

77 Zn 1.372414

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.021996

2 C 0.308669

3 N -0.706255

4 C 0.308669

5 C -0.021996

6 C -0.149008

7 C 0.308669

8 N -0.706255

9 C 0.308669

10 C -0.021996

11 C -0.021996

12 C -0.149008

13 C 0.308669

14 C -0.021996

15 C -0.021996

16 C 0.308669

17 N -0.706255

18 C -0.149008

19 C 0.308669

20 C -0.021996

21 C -0.021996

22 C 0.308669

23 N -0.706255

24 C -0.149008

25 C -0.105849

26 C 0.012342

27 C 0.007981

28 C 0.004019

29 C 0.007981

30 C 0.012342

31 C 0.004019

32 C 0.007981

33 C 0.012342

34 C -0.105849

35 C 0.012342

36 C 0.007981

37 C -0.105849

38 C 0.012342

39 C 0.007981

40 C 0.004019

41 C 0.007981

42 C 0.012342

43 C -0.105849

44 C 0.012342

45 C 0.007981

46 C 0.004019

47 C 0.007981

48 C 0.012342

77 Zn 1.372414

Electronic spatial extent (au): <R\*\*2>= 33352.9763

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

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

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

XX= -248.6475 YY= -248.6475 ZZ= -276.6355

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 9.3294 YY= 9.3294 ZZ= -18.6587

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

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

XXY= 0.0000 XXZ= 89.9106 XZZ= 0.0000 YZZ= 0.0000

YYZ= -89.9106 XYZ= 0.0000

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

XXXX= -21528.0535 YYYY= -21528.0535 ZZZZ= -1080.9899 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -5779.9006 XXZZ= -3834.9819 YYZZ= -3834.9819

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 5.738269430807D+03 E-N=-1.615865211036D+04 KE= 2.020706235307D+03

Symmetry A1 KE= 5.778493057935D+02

Symmetry A2 KE= 4.453814231484D+02

Symmetry B1 KE= 4.987377531825D+02

Symmetry B2 KE= 4.987377531825D+02

Leave Link 601 at Thu Sep 5 22:07:21 2019, MaxMem= 1342177280 cpu: 53.3

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

Test job not archived.

1\1\GINC-K251\SP\RB3LYP TD-FC\GenECP\C44H28N4Zn1\Z5105842\05-Sep-2019\

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

icaldispersion=gd3bj IOp(9/40=3)\\ZnTPP0td\\0,1\C,0,-0.681484,4.269157

,0.164086\C,0,-1.110541,2.890129,0.035503\N,0,0.,2.090529,-0.027459\C,

0,1.110541,2.890129,0.035503\C,0,0.681484,4.269157,0.164086\C,0,2.4521

83,2.452183,0.\C,0,2.890129,1.110541,-0.035503\N,0,2.090529,0.,0.02745

9\C,0,2.890129,-1.110541,-0.035503\C,0,4.269157,-0.681484,-0.164086\C,

0,4.269157,0.681484,-0.164086\C,0,-2.452183,2.452183,0.\C,0,-2.890129,

1.110541,-0.035503\C,0,-4.269157,0.681484,-0.164086\C,0,-4.269157,-0.6

81484,-0.164086\C,0,-2.890129,-1.110541,-0.035503\N,0,-2.090529,0.,0.0

27459\C,0,-2.452183,-2.452183,0.\C,0,-1.110541,-2.890129,0.035503\C,0,

-0.681484,-4.269157,0.164086\C,0,0.681484,-4.269157,0.164086\C,0,1.110

541,-2.890129,0.035503\N,0,0.,-2.090529,-0.027459\C,0,2.452183,-2.4521

83,0.\C,0,3.508242,3.508242,0.\C,0,3.621357,4.405038,-1.069674\C,0,4.6

07485,5.388753,-1.071137\C,0,5.493806,5.493806,0.\C,0,5.388753,4.60748

5,1.071137\C,0,4.405038,3.621357,1.069674\C,0,-5.493806,5.493806,0.\C,

0,-4.607485,5.388753,-1.071137\C,0,-3.621357,4.405038,-1.069674\C,0,-3

.508242,3.508242,0.\C,0,-4.405038,3.621357,1.069674\C,0,-5.388753,4.60

7485,1.071137\C,0,3.508242,-3.508242,0.\C,0,4.405038,-3.621357,1.06967

4\C,0,5.388753,-4.607485,1.071137\C,0,5.493806,-5.493806,0.\C,0,4.6074

85,-5.388753,-1.071137\C,0,3.621357,-4.405038,-1.069674\C,0,-3.508242,

-3.508242,0.\C,0,-4.405038,-3.621357,1.069674\C,0,-5.388753,-4.607485,

1.071137\C,0,-5.493806,-5.493806,0.\C,0,-4.607485,-5.388753,-1.071137\

C,0,-3.621357,-4.405038,-1.069674\H,0,-1.330917,5.125618,0.259828\H,0,

1.330917,5.125618,0.259828\H,0,5.125618,-1.330917,-0.259828\H,0,5.1256

18,1.330917,-0.259828\H,0,-5.125618,1.330917,-0.259828\H,0,-5.125618,-

1.330917,-0.259828\H,0,-1.330917,-5.125618,0.259828\H,0,1.330917,-5.12

5618,0.259828\H,0,2.936967,4.323214,-1.90704\H,0,4.684584,6.071446,-1.

91098\H,0,6.260992,6.260992,0.\H,0,6.071446,4.684584,1.91098\H,0,4.323

214,2.936967,1.90704\H,0,-6.260992,6.260992,0.\H,0,-4.684584,6.071446,

-1.91098\H,0,-2.936967,4.323214,-1.90704\H,0,-4.323214,2.936967,1.9070

4\H,0,-6.071446,4.684584,1.91098\H,0,4.323214,-2.936967,1.90704\H,0,6.

071446,-4.684584,1.91098\H,0,6.260992,-6.260992,0.\H,0,4.684584,-6.071

446,-1.91098\H,0,2.936967,-4.323214,-1.90704\H,0,-4.323214,-2.936967,1

.90704\H,0,-6.071446,-4.684584,1.91098\H,0,-6.260992,-6.260992,0.\H,0,

-4.684584,-6.071446,-1.91098\H,0,-2.936967,-4.323214,-1.90704\Zn,0,0.,

0.,0.\\Version=ES64L-G09RevD.01\State=1-A1\HF=-1978.9047638\RMSD=2.710

e-09\PG=D02D [O(Zn1),2SGD(N2),X(C44H28)]\\@

A BIRD IN THE HAND IS SAFER THAN ONE OVERHEAD.

-- NEWTON'S SEVENTH LAW

Job cpu time: 0 days 4 hours 30 minutes 48.1 seconds.

File lengths (MBytes): RWF= 3666 Int= 0 D2E= 0 Chk= 343 Scr= 2

Normal termination of Gaussian 09 at Thu Sep 5 22:07:24 2019.