Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Optical and magnetic properties of antiaromatic porphyrinoids

Rashid R. Valiev,[*,†] Heike Fliegl,[*,‡] and Dage Sundholm[*,¶]

†*University of Helsinki, Department of Chemistry, P.O. Box 55 (A.I. Virtanens plats 1), FIN-00014 Finland; Russian Federation, Tomsk State University, Tomsk, Lenina Avenue 36*

‡*Centre for Theoretical and Computational Chemistry (CTCC), Department of Chemistry, University of Oslo, P.O.Box 1033 Blindern, 0315 Oslo, Norway*

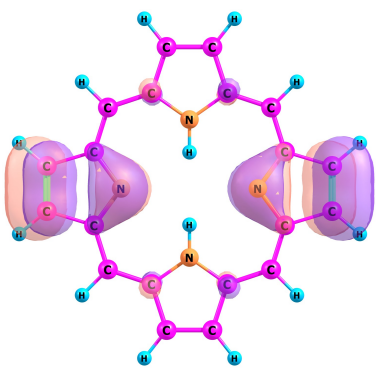
¶*University of Helsinki, Department of Chemistry, P.O. Box 55 (A.I. Virtanens plats 1), FIN-00014 Helsinki, Finland*

E-mail: valievrashid@mail.ru; Heike.Fliegl@kjemi.uio.no; Dage.Sundholm@helsinki.fi

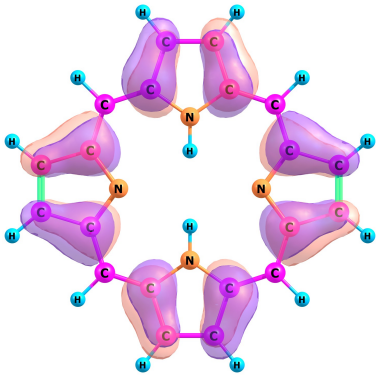
Contents

1 The frontier MOs obtained at the B3LYP level

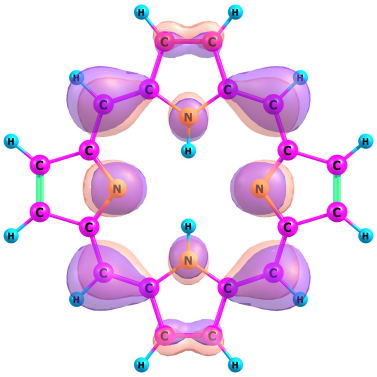
1.1 H_2P



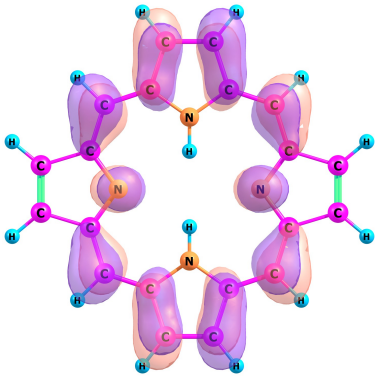
HOMO-2(B_{2G})



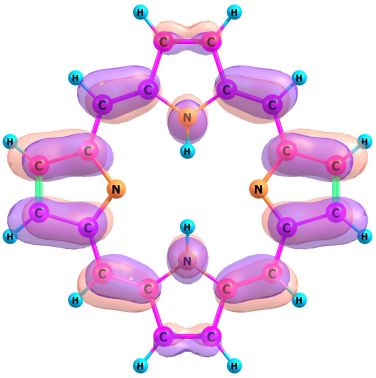
HOMO-1(A_U)



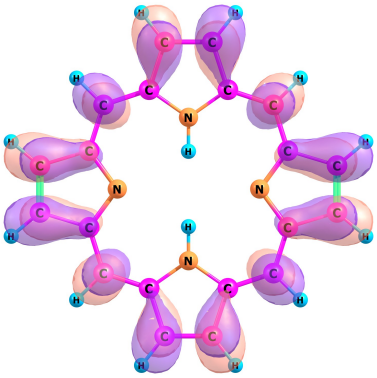
HOMO(B_{1U})



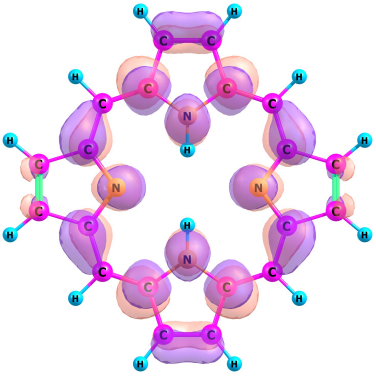
LUMO(B_{2G})



LUMO+1(B_{3G})



LUMO+2(A_U)



LUMO+3(B_{1U})

Figure 1: Plots of the frontier molecular orbitals of compound I.

1.2 I

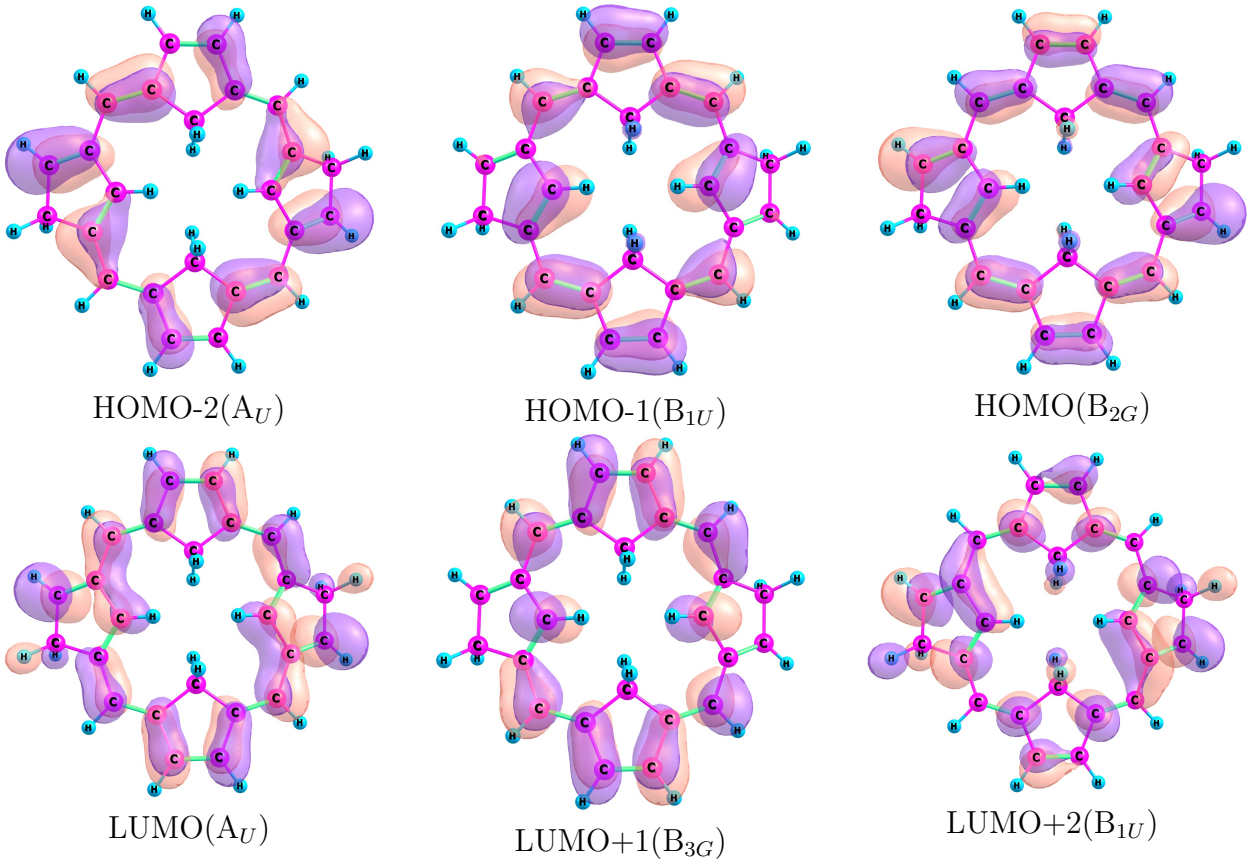


Figure 2: Plots of the frontier molecular orbitals of compound I.

1.3 II

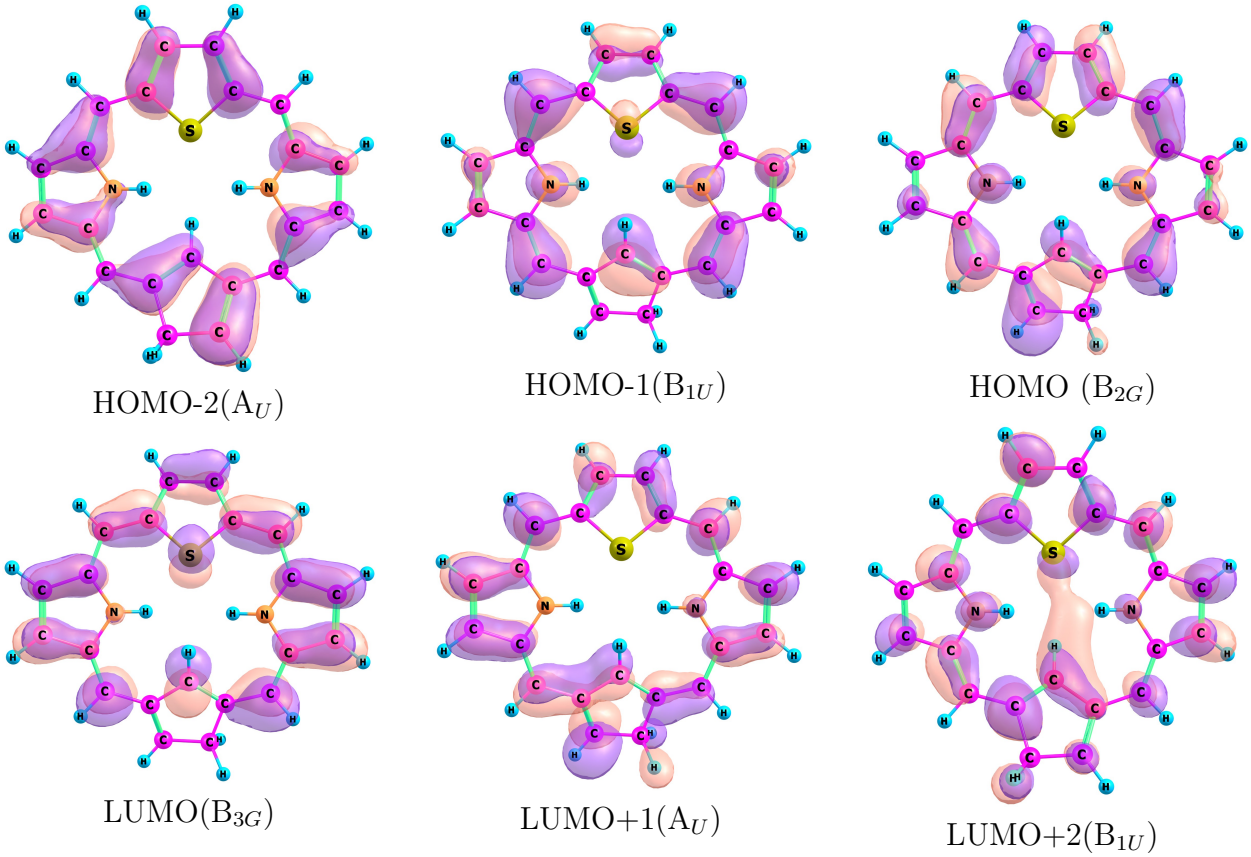


Figure 3: Plots of the frontier molecular orbitals of compound II.

1.4 III

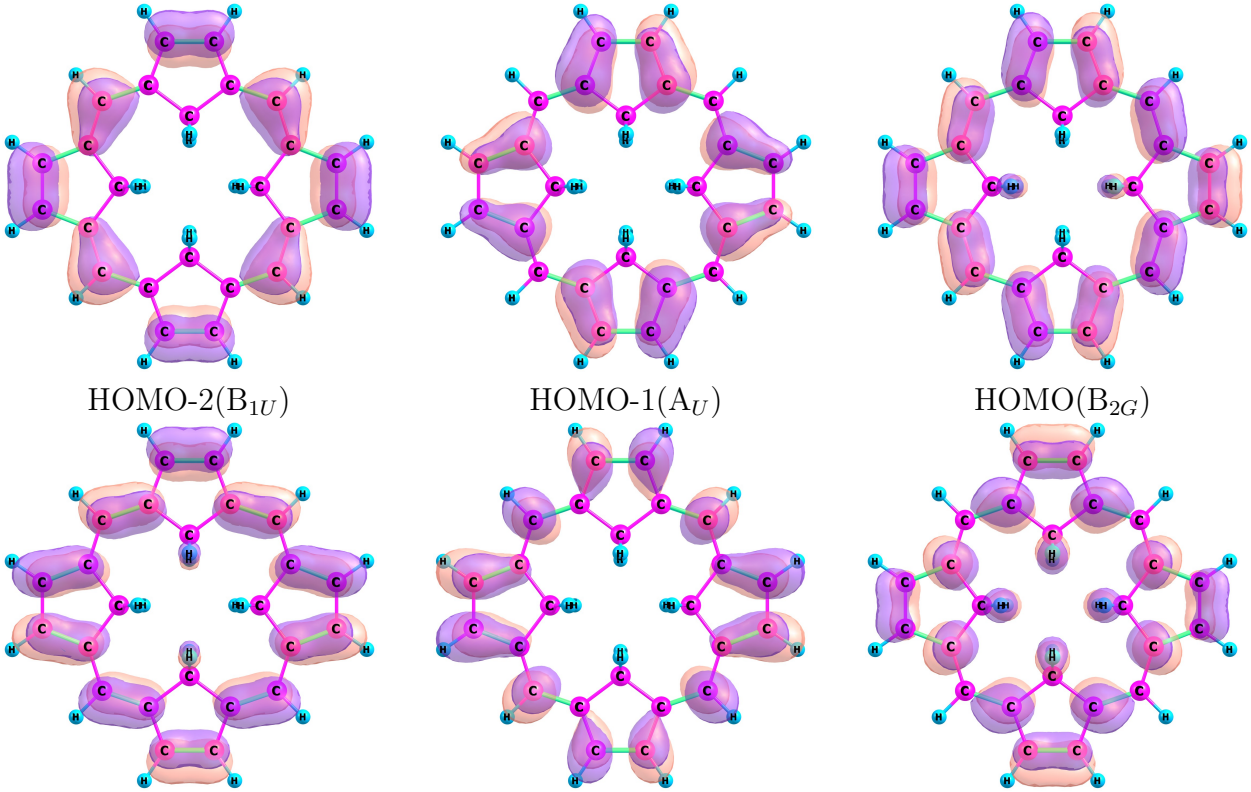


Figure 4: Plots of the frontier molecular orbitals of compound III.

1.5 IV

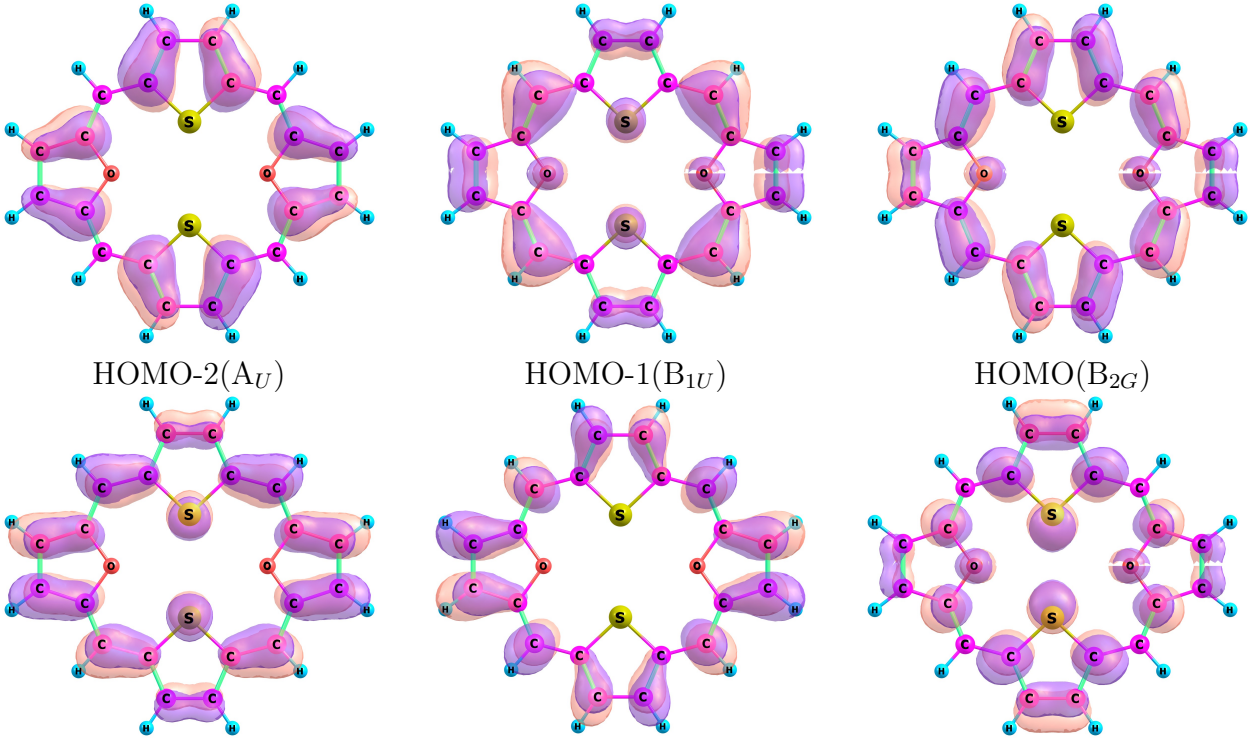
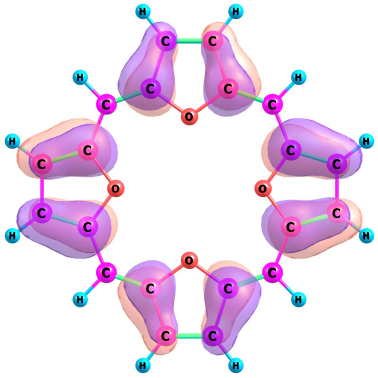
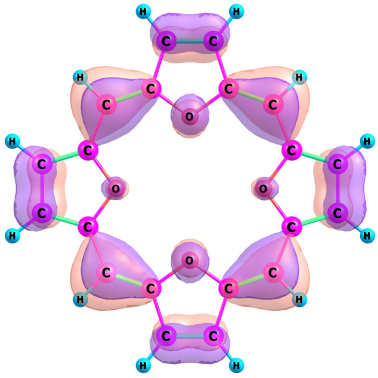


Figure 5: Plots of the frontier molecular orbitals of compound IV.

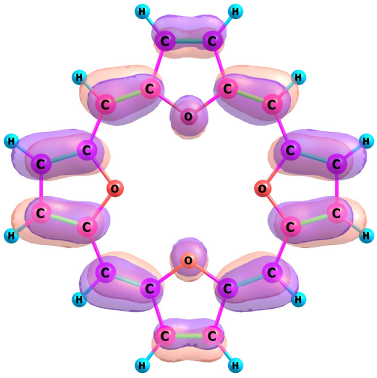
1.6 V



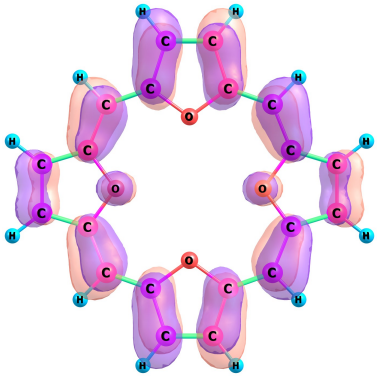
HOMO-2(A_U)



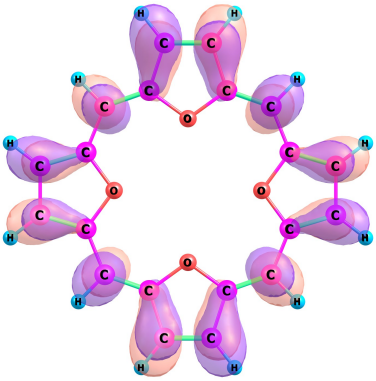
HOMO-1(B_{1U})



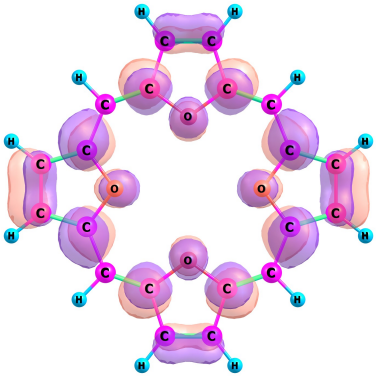
HOMO(B_{2G})



LUMO(B_{3G})



LUMO+1(A_U)



LUMO+2(B_{1U})

Figure 6: Plots of the frontier molecular orbitals of compound V.

1.7 VI

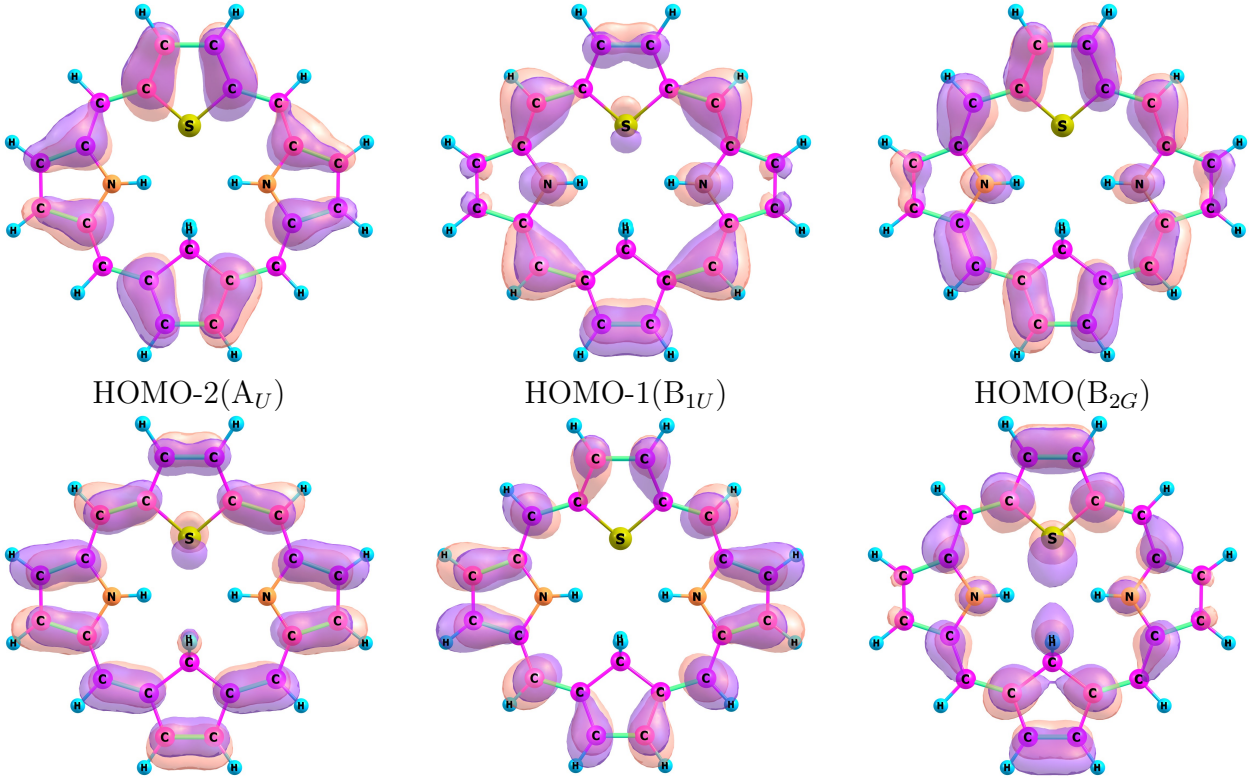


Figure 7: Plots of the frontier molecular orbitals of compound VI.

1.8 VII

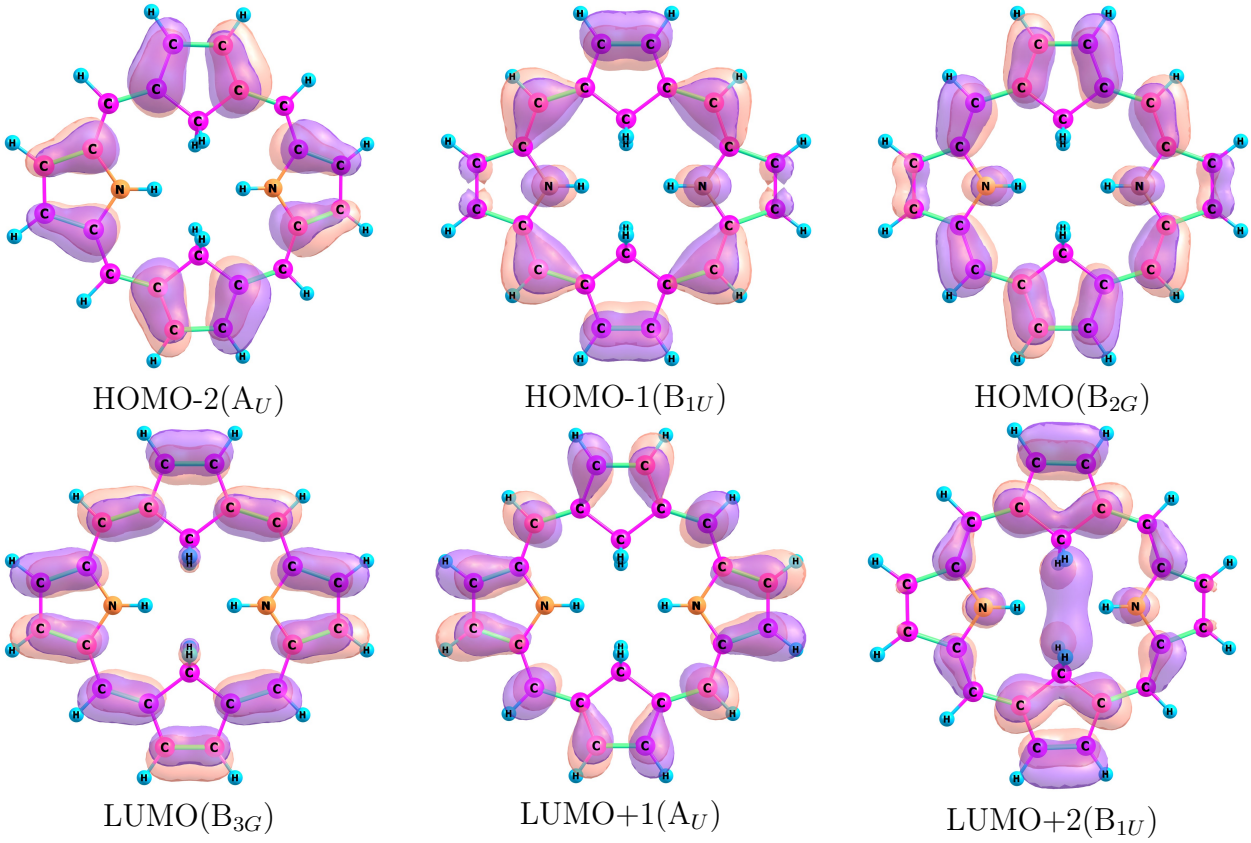


Figure 8: Plots of the frontier molecular orbitals of compound VII.

2 Largest contributions to the $S_0 \rightarrow S_n$ transitions

The largest contributions to the $S_0 \rightarrow S_1$-S_5 electronic transitions have been calculated at the TDDFT/B3LYP/def2-TZVP level. The weights are given in parenthesis.

2.1 I compound

```
state | % transition(weight)
================================
1         H->L+1(0.70)
2         H->L(0.67)
3         H-1->L(0.70)
4         H-2->L(-0.42);H->L+2(0.56)
5         H-2->L+1(-0.41);H->L+1(0.49)
```

2.2 II compound

```
state | % transition(weight)
==============================
1        H->L(0.71)
2        H->L+1(0.88)
3        H-2->L(0.50);H-1->L+1(-0.45)
4        H-1->L(0.56);H-1->L(0.36)
5        H-1->L+1(-0.42);H->L+1(0.46)
```

2.3 III compound

```
state | % transition(weight)
==============================
1        H->L(0.71)
2        H-1->L(0.56);H->L+2(0.43)
3        H-2->L(0.56);H->L+1(0.42)
4        H-1->L(-0.43);H->L+2(0.56)
5        H-2->L(0.54);H->L+1(-0.46)
```

2.4 IV compound

```
state | % transition(weight)
==============================
1        H->L(0.71)
2        H->L+1(0.59);H->L+1(-0.38)
3        H-2->L(0.54);H->L+2(0.45)
4        H-3->L(0.70)
5        H-4->L(-0.45);H-1->L+1(0.46)
```

2.5 V compound

```
state | % transition(weight)
==============================
1        H->L(0.71)
2        H->L+1(0.59);H-1->L(-0.39)
3        H-2->L(0.59);H->L+2(-0.39)
4        H-1->L(0.58);H->L+1(0.39)
5        H-2->L(0.40);H->L+2(0.58)
```

2.6 VI compound

```
state | % transition(weight)
==============================
1        H->L(0.71)
2        H-1->L(-0.45);H->L+1(0.54)
3        H-2->L(0.51);H->L+2(-0.49)
4        H-1->L(0.53);H->L+1(0.44)
5        H-2->L(0.48);H->L+2(0.50)
```

2.7 VII compound

```
state | % transition(weight)
==============================
1        H->L(0.71)
2        H-1->L(0.44);H->L+1(0.56)
3        H-2->L(0.47);H->L+2(0.52)
4        H-2->L(0.50);H->L+2(-0.43)
5        H-2->L(0.55);H->L+2(-0.44)
```

3 Transition moments for $\mathbf{S}_0 \rightarrow \mathbf{S}_n$, $n = 1 - 5$

3.1 I compound

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

state	X	Y	Z	Dip. S.	Osc.
1	0.0003	-0.0005	0.0372	0.0014	0.0001
2	-1.9676	-0.3787	0.0003	4.0150	0.2535
3	-0.0010	0.0002	-0.0249	0.0006	0.0000
4	0.0004	-0.0001	-0.0388	0.0015	0.0001
5	1.4913	1.1100	0.0002	3.4561	0.2957

3.2 II compound

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

state	X	Y	Z	Dip. S.	Osc.

1	-0.7775	-0.1710	0.0193	0.6341	0.0203
2	0.1800	-1.1670	-0.0574	1.3976	0.0755
3	0.3777	0.7788	0.0097	0.7493	0.0569
4	1.1184	-2.9445	-0.0360	9.9221	0.7761
5	0.8064	0.4418	0.0209	0.8458	0.0687

3.3 III compound

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

state	X	Y	Z	Dip. S.	Osc.
1	0.0001	0.0003	0.0001	0.0000	0.0000
2	-0.5430	-0.0005	0.0000	0.2949	0.0195
3	-0.0006	0.3959	0.0001	0.1568	0.0104
4	3.3745	0.0014	0.0000	11.3874	0.9956
5	0.0021	-3.8062	-0.0005	14.4868	1.2986

3.4 IV compound

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

state	X	Y	Z	Dip. S.	Osc.
1	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.8597	0.7391	0.0465
3	0.0003	0.6127	0.0000	0.3753	0.0274
4	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	2.2358	4.9988	0.4303

3.5 V compound

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

state	X	Y	Z	Dip. S.	Osc.
1	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.9905	0.9811	0.0618
3	0.0000	1.0094	0.0000	1.0188	0.0770
4	0.0000	0.0000	3.8724	14.9954	1.3729
5	0.0003	3.5153	0.0000	12.3573	1.2416

3.6 VI compound

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

state	X	Y	Z	Dip. S.	Osc.
1	0.3532	-0.0006	0.0001	0.1248	0.0020
2	-0.0001	0.4015	-0.0024	0.1612	0.0092
3	-0.3882	-0.0002	0.0000	0.1507	0.0104
4	0.0001	3.2962	0.0561	10.8680	0.8792
5	-2.9507	-0.0007	0.0000	8.7068	0.7489

3.7 VII compound

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

state	X	Y	Z	Dip. S.	Osc.
1	0.0001	0.0017	-0.0001	0.0000	0.0000
2	0.0001	0.4693	0.0000	0.2203	0.0121
3	-0.2665	0.0001	0.0002	0.0710	0.0046
4	-2.7118	-0.0007	-0.0009	7.3538	0.5960
5	0.0010	-3.6641	-0.0001	13.4254	1.1076

4 CC2 energies and transition moments

4.1 I

```
================================================================================
  |  Transition                                                  model: CC2
  |    number, symmetry, multiplicity:    1 a    1
  |    frequency :   0.1061019429 a.u.     2.88718 e.V.     23286.7 rcm
  +==============================================================================

     +-----------+---------------------+
     | operator  | transition strength |
     +-----------+---------------------+
     | xangmom   |          0.00000076 |
     | yangmom   |          0.00000000 |
     | zangmom   |         20.38992504 |
     | xdiplen   |          0.00000024 |
     | ydiplen   |          0.00000077 |
     | zdiplen   |          0.00088714 |
     +-----------+---------------------+

       oscillator strength (length gauge)   :      0.00006282
       rotator strength (length gauge)      :     -0.06859045 a.u.
       Rotator strength (length gauge)      :    -32.33653226 10^(-40)*erg*cm^3
```

```
+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    2 a    1
|    frequency :   0.1162134326 a.u.     3.16233 e.V.     25505.9 rcm
+====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.01210604    |
   | yangmom   |       0.00832721    |
   | zangmom   |       0.00000188    |
   | xdiplen   |       7.23306237    |
   | ydiplen   |       0.37163500    |
   | zdiplen   |       0.00000001    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.58917866
     rotator strength (length gauge)      :      0.11858420 a.u.
     Rotator strength (length gauge)      :     55.90576600 10^(-40)*erg*cm^3


+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1323912587 a.u.     3.60255 e.V.     29056.5 rcm
+====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000107    |
   | yangmom   |       0.00000000    |
   | zangmom   |       4.85088863    |
   | xdiplen   |       0.00000004    |
   | ydiplen   |       0.00000008    |
   | zdiplen   |       0.00002023    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.00000180
     rotator strength (length gauge)      :     -0.00504617 a.u.
     Rotator strength (length gauge)      :     -2.37898412 10^(-40)*erg*cm^3


+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1430732520 a.u.     3.89322 e.V.     31400.9 rcm
+====================================================================

   +-----------+---------------------+
   | operator  |transition strength |
   +-----------+---------------------+
   | xangmom   |      0.00000003    |
   | yangmom   |      0.00000004    |
   | zangmom   |      0.07377303    |
   | xdiplen   |      0.00000023    |
   | ydiplen   |      0.00000003    |
   | zdiplen   |      0.00543574    |
   +-----------+---------------------+
```

```
     oscillator strength (length gauge)   :      0.00051850
     rotator strength (length gauge)      :      0.01014511 a.u.
     Rotator strength (length gauge)      :      4.78284703 10^(-40)*erg*cm^3

+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1485774389 a.u.     4.04300 e.V.     32609.0 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00025357    |
   | yangmom   |       0.00084491    |
   | zangmom   |       0.00000008    |
   | xdiplen   |       1.01174037    |
   | ydiplen   |       1.43223584    |
   | zdiplen   |       0.00000008    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.24207983
     rotator strength (length gauge)      :      0.00981429 a.u.
     Rotator strength (length gauge)      :      4.62688394 10^(-40)*erg*cm^3
```

4.2 II

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    1 a    1
|    frequency :   0.0597140289 a.u.     1.62490 e.V.     13105.7 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00031916    |
   | yangmom   |       0.00607798    |
   | zangmom   |      16.57097015    |
   | xdiplen   |       0.86478586    |
   | ydiplen   |       0.06006449    |
   | zdiplen   |       0.00038919    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.03683319
```

```
     rotator strength (length gauge)      :     -0.02289560 a.u.
     Rotator strength (length gauge)      :    -10.79398667 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                                 model: CC2
|    number, symmetry, multiplicity:    2 a    1
|    frequency :   0.0933733131 a.u.     2.54082 e.V.     20493.1 rcm
+=====================================================================
```

operator	transition strength
xangmom	0.00684723
yangmom	0.00029957
zangmom	0.18096197
xdiplen	0.06910316
ydiplen	2.34788073
zdiplen	0.00404816

```
     oscillator strength (length gauge)   :      0.15070652

     rotator strength (length gauge)      :     -0.01165683 a.u.
     Rotator strength (length gauge)      :     -5.49553890 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                                 model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1232134439 a.u.     3.35281 e.V.     27042.2 rcm
+=====================================================================
```

operator	transition strength
xangmom	0.00024344
yangmom	0.00023003
zangmom	0.01989246
xdiplen	0.59249783
ydiplen	10.08498341
zdiplen	0.00043121

```
   +-------------------------------+

     oscillator strength (length gauge)   :      0.87710824

     rotator strength (length gauge)      :      0.01596203 a.u.
     Rotator strength (length gauge)      :      7.52519602 10^(-40)*erg*cm^3


+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1290522525 a.u.     3.51169 e.V.     28323.7 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00151364    |
   | yangmom   |       0.00188965    |
   | zangmom   |       0.58134608    |
   | xdiplen   |       0.44394769    |
   | ydiplen   |       0.26539155    |
   | zdiplen   |       0.00000402    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.06102754

     rotator strength (length gauge)      :     -0.02491080 a.u.
     Rotator strength (length gauge)      :    -11.74403665 10^(-40)*erg*cm^3


+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1368508243 a.u.     3.72390 e.V.     30035.3 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000767    |
   | yangmom   |       0.00003573    |
   | zangmom   |       0.13207073    |
```

```
   | xdiplen   |       1.41984607    |
   | ydiplen   |       0.01868064    |
   | zdiplen   |       0.00000980    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.13124327

     rotator strength (length gauge)      :     -0.00071840 a.u.
     Rotator strength (length gauge)      :     -0.33868286 10^(-40)*erg*cm^3
```

4.3 III

```
 +=====================================================================
  |  Transition                                              model: CC2
  |    number, symmetry, multiplicity:    1 a    1
  |    frequency :   0.0575370637 a.u.     1.56566 e.V.     12627.9 rcm
 +=====================================================================

    +-----------+---------------------+
    | operator  | transition strength |
    +-----------+---------------------+
    | xangmom   |       0.00000000    |
    | yangmom   |       0.00000053    |
    | zangmom   |      27.10475280    |
    | xdiplen   |       0.00000000    |
    | ydiplen   |       0.00000000    |
    | zdiplen   |       0.00000001    |
    +-----------+---------------------+

     oscillator strength (length gauge)   :      0.00000000

     rotator strength (length gauge)      :      0.00027786 a.u.
     Rotator strength (length gauge)      :      0.13099337 10^(-40)*erg*cm^3


 +=====================================================================
  |  Transition                                              model: CC2
  |    number, symmetry, multiplicity:    2 a    1
```

```
|    frequency :   0.1195888374 a.u.     3.25418 e.V.     26246.7 rcm
+=====================================================================

   +-----------+--------------------+
   | operator  | transition strength |
   +-----------+--------------------+
   | xangmom   |       0.00000003    |
   | yangmom   |       0.00000232    |
   | zangmom   |       0.00000001    |
   | xdiplen   |       0.58425621    |
   | ydiplen   |       0.00000019    |
   | zdiplen   |       0.00000000    |
   +-----------+--------------------+

     oscillator strength (length gauge)   :      0.04658036

     rotator strength (length gauge)      :      0.00006518 a.u.
     Rotator strength (length gauge)      :      0.03072713 10^(-40)*erg*cm^3



+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1243239218 a.u.     3.38303 e.V.     27285.9 rcm
+=====================================================================

   +-----------+--------------------+
   | operator  | transition strength |
   +-----------+--------------------+
   | xangmom   |       0.00000042    |
   | yangmom   |       0.00000006    |
   | zangmom   |       0.00000001    |
   | xdiplen   |       0.00000021    |
   | ydiplen   |       0.42888550    |
   | zdiplen   |       0.00000002    |
   +-----------+--------------------+

     oscillator strength (length gauge)   :      0.03554717

     rotator strength (length gauge)      :     -0.00008335 a.u.
     Rotator strength (length gauge)      :     -0.03929354 10^(-40)*erg*cm^3
```

```
+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1451873739 a.u.     3.95075 e.V.     31864.9 rcm
+====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000091    |
   | yangmom   |       0.00003626    |
   | zangmom   |       0.00000012    |
   | xdiplen   |      12.98983710    |
   | ydiplen   |       0.00000226    |
   | zdiplen   |       0.00000000    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      1.25730711

     rotator strength (length gauge)      :      0.00172756 a.u.
     Rotator strength (length gauge)      :      0.81444864 10^(-40)*erg*cm^3



+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1496657758 a.u.     4.07261 e.V.     32847.8 rcm
+====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00001387    |
   | yangmom   |       0.00000095    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000301    |
   | ydiplen   |      15.81047982    |
   | zdiplen   |       0.00000037    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      1.57752549

     rotator strength (length gauge)      :     -0.00195386 a.u.
     Rotator strength (length gauge)      :     -0.92113451 10^(-40)*erg*cm^3
```

4.4 IV

```
+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    1 a    1
|    frequency :   0.0459965876 a.u.     1.25163 e.V.     10095.1 rcm
+====================================================================

   +-----------+--------------------+
   | operator  | transition strength |
   +-----------+--------------------+
   | xangmom   |      26.71932112    |
   | yangmom   |       0.00000250    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000000    |
   | ydiplen   |       0.00000000    |
   | zdiplen   |       0.00000000    |
   +-----------+--------------------+

     oscillator strength (length gauge)   :      0.00000000

     rotator strength (length gauge)      :     -0.00000000 a.u.
     Rotator strength (length gauge)      :     -0.00000000 10^(-40)*erg*cm^3



+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    2 a    1
|    frequency :   0.1132936125 a.u.     3.08288 e.V.     24865.1 rcm
+====================================================================

   +-----------+--------------------+
   | operator  |transition strength |
   +-----------+--------------------+
   | xangmom   |      0.00000000    |
   | yangmom   |      0.00000000    |
   | zangmom   |      0.00000000    |
```

```
   | xdiplen   |      0.00000000    |
   | ydiplen   |      0.00000000    |
   | zdiplen   |      1.88409167    |
   +-----------+--------------------+

     oscillator strength (length gauge)   :      0.14230370

     rotator strength (length gauge)      :     -0.00000000 a.u.
     Rotator strength (length gauge)      :     -0.00000000 10^(-40)*erg*cm^3


+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1241814995 a.u.     3.37915 e.V.     27254.7 rcm
+=====================================================================

   +-----------+--------------------+
   | operator  | transition strength |
   +-----------+--------------------+
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00000000    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000016    |
   | ydiplen   |       0.88546204    |
   | zdiplen   |       0.00000000    |
   +-----------+--------------------+

     oscillator strength (length gauge)   :      0.07330535

     rotator strength (length gauge)      :      0.00000000 a.u.
     Rotator strength (length gauge)      :      0.00000000 10^(-40)*erg*cm^3


+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1400184237 a.u.     3.81010 e.V.     30730.5 rcm
+=====================================================================

   +-----------+--------------------+
   | operator  | transition strength |
   +-----------+--------------------+
```

```
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00000000    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000000    |
   | ydiplen   |       0.00000000    |
   | zdiplen   |      10.14852356    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.94732018

     rotator strength (length gauge)      :     -0.00000000 a.u.
     Rotator strength (length gauge)      :     -0.00000000 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1525411586 a.u.     4.15086 e.V.     33478.9 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00000000    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000160    |
   | ydiplen   |      12.40834038    |
   | zdiplen   |       0.00000000    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      1.26185524

     rotator strength (length gauge)      :     -0.00000000 a.u.
     Rotator strength (length gauge)      :     -0.00000001 10^(-40)*erg*cm^3
```

4.5 V

```
+=====================================================================
|  Transition                                              model: CC2
```

```
|    number, symmetry, multiplicity:    1 a    1
|    frequency :   0.0464723715 a.u.     1.26458 e.V.     10199.5 rcm
+=====================================================================
```

operator	transition strength
xangmom	27.06092542
yangmom	0.00000013
zangmom	0.00000000
xdiplen	0.00000000
ydiplen	0.00000000
zdiplen	0.00000000

```
  oscillator strength (length gauge)   :      0.00000000

  rotator strength (length gauge)      :      0.00000000 a.u.
  Rotator strength (length gauge)      :      0.00000002 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                                 model: CC2
|    number, symmetry, multiplicity:    2 a    1
|    frequency :   0.1174462494 a.u.     3.19588 e.V.     25776.5 rcm
+=====================================================================
```

operator	transition strength
xangmom	0.00000000
yangmom	0.00000000
zangmom	0.00000000
xdiplen	0.00000000
ydiplen	0.00000000
zdiplen	3.27924030

```
  oscillator strength (length gauge)   :      0.25675632

  rotator strength (length gauge)      :      0.00000000 a.u.
  Rotator strength (length gauge)      :      0.00000001 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1346080404 a.u.     3.66287 e.V.     29543.0 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00000000    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000001    |
   | ydiplen   |       2.39116242    |
   | zdiplen   |       0.00000000    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.21457979

     rotator strength (length gauge)      :      0.00000000 a.u.
     Rotator strength (length gauge)      :      0.00000004 10^(-40)*erg*cm^3



+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1482446810 a.u.     4.03394 e.V.     32535.9 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00000000    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000000    |
   | ydiplen   |       0.00000000    |
   | zdiplen   |      13.78795740    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      1.36266090

     rotator strength (length gauge)      :     -0.00000000 a.u.
```

```
     Rotator strength (length gauge)      :     -0.00000022 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1680603085 a.u.     4.57315 e.V.     36885.0 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00000000    |
   | zangmom   |       0.00000000    |
   | xdiplen   |       0.00000009    |
   | ydiplen   |      12.01706876    |
   | zdiplen   |       0.00000000    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      1.34639487

     rotator strength (length gauge)      :     -0.00000000 a.u.
     Rotator strength (length gauge)      :     -0.00000029 10^(-40)*erg*cm^3
```

4.6 VI

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    1 a    1
|    frequency :   0.0365210557 a.u.     0.99379 e.V.      8015.4 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000001    |
```

```
   | yangmom   |       0.00248088    |
   | zangmom   |      25.38259640    |
   | xdiplen   |       0.17234065    |
   | ydiplen   |       0.00000076    |
   | zdiplen   |       0.00000001    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.00419606

     rotator strength (length gauge)      :     -0.00027361 a.u.
     Rotator strength (length gauge)      :     -0.12898942 10^(-40)*erg*cm^3



+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    2 a    1
|    frequency :   0.1030312086 a.u.     2.80362 e.V.     22612.7 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00268213    |
   | yangmom   |       0.00000001    |
   | zangmom   |       0.00000001    |
   | xdiplen   |       0.00000003    |
   | ydiplen   |       0.10153098    |
   | zdiplen   |       0.00001328    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.00697482

     rotator strength (length gauge)      :      0.00001407 a.u.
     Rotator strength (length gauge)      :      0.00663472 10^(-40)*erg*cm^3



+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1185856634 a.u.     3.22688 e.V.     26026.5 rcm
+=====================================================================

   +-----------+---------------------+
```

```
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00000000    |
   | yangmom   |       0.00013593    |
   | zangmom   |       0.00047624    |
   | xdiplen   |       0.12681448    |
   | ydiplen   |       0.00000004    |
   | zdiplen   |       0.00000000    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      0.01002559

     rotator strength (length gauge)      :     -0.00000092 a.u.
     Rotator strength (length gauge)      :     -0.00043360 10^(-40)*erg*cm^3


+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1264328337 a.u.     3.44041 e.V.     27748.8 rcm
+=====================================================================

   +-----------+---------------------+
   | operator  | transition strength |
   +-----------+---------------------+
   | xangmom   |       0.00176237    |
   | yangmom   |       0.00000006    |
   | zangmom   |       0.00000034    |
   | xdiplen   |       0.00000057    |
   | ydiplen   |      12.64649383    |
   | zdiplen   |       0.00375466    |
   +-----------+---------------------+

     oscillator strength (length gauge)   :      1.06627122

     rotator strength (length gauge)      :      0.00041542 a.u.
     Rotator strength (length gauge)      :      0.19584791 10^(-40)*erg*cm^3

+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1409509788 a.u.     3.83547 e.V.     30935.2 rcm
+=====================================================================
```

operator	transition strength
xangmom	0.00000002
yangmom	0.04591296
zangmom	0.01967016
xdiplen	9.76134130
ydiplen	0.00000001
zdiplen	0.00000000

oscillator strength (length gauge) : 0.91724707

rotator strength (length gauge) : -0.00023497 a.u.
Rotator strength (length gauge) : -0.11077428 10^(-40)*erg*cm^3

4.7 VII

Transition		model: CC2
number, symmetry, multiplicity:	1 a 1	
frequency : 0.0293918872 a.u.	0.79979 e.V.	6450.8 rcm

operator	transition strength
xangmom	0.00000366
yangmom	0.00000002
zangmom	27.71189842
xdiplen	0.00000000
ydiplen	0.00001002
zdiplen	0.00000000

oscillator strength (length gauge) : 0.00000020

rotator strength (length gauge) : 0.00016896 a.u.

```
     Rotator strength (length gauge)      :      0.07965711 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    2 a    1
|    frequency :   0.1013706290 a.u.     2.75844 e.V.     22248.3 rcm
+=====================================================================
```

operator	transition strength
xangmom	0.00029502
yangmom	0.00000000
zangmom	0.00000689
xdiplen	0.00000001
ydiplen	0.24404329
zdiplen	0.00000000

```
     oscillator strength (length gauge)   :      0.01649255

     rotator strength (length gauge)      :     -0.00001337 a.u.
     Rotator strength (length gauge)      :     -0.00630542 10^(-40)*erg*cm^3
```

```
+=====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    3 a    1
|    frequency :   0.1115284171 a.u.     3.03484 e.V.     24477.7 rcm
+=====================================================================
```

operator	transition strength
xangmom	0.00000000
yangmom	0.00028827
zangmom	0.00000033
xdiplen	0.04781286
ydiplen	0.00000016
zdiplen	0.00000007

```
     oscillator strength (length gauge)   :      0.00355501

     rotator strength (length gauge)      :     -0.00000546 a.u.
     Rotator strength (length gauge)      :     -0.00257620 10^(-40)*erg*cm^3
```

```
+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    4 a    1
|    frequency :   0.1289423356 a.u.     3.50870 e.V.     28299.6 rcm
+====================================================================
```

operator	transition strength
xangmom	0.00255622
yangmom	0.00000006
zangmom	0.00001236
xdiplen	0.00000061
ydiplen	15.22129953
zdiplen	0.00000001

```
     oscillator strength (length gauge)   :      1.30844666

     rotator strength (length gauge)      :     -0.00050095 a.u.
     Rotator strength (length gauge)      :     -0.23616773 10^(-40)*erg*cm^3
```

```
+====================================================================
|  Transition                                              model: CC2
|    number, symmetry, multiplicity:    5 a    1
|    frequency :   0.1319291434 a.u.     3.58997 e.V.     28955.1 rcm
+====================================================================
```

operator	transition strength
xangmom	0.00000004
yangmom	0.00008542
zangmom	0.00000002
xdiplen	5.66355239
ydiplen	0.00000002

```
| zdiplen   |       0.00000054    |
+-----------+---------------------+

  oscillator strength (length gauge)   :      0.49812512

  rotator strength (length gauge)      :      0.00022600 a.u.
  Rotator strength (length gauge)      :      0.10654438 10^(-40)*erg*cm^3
```