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

o-Benzyne fragmentation and isomerization pathways. A CASPT2 study.

Giovanni Ghigo, Andrea Maranzana, Glauco Tonachini*

Supplementary Information

Determination of ZPE scale factor.

The calculation of thermochemical data requires the proper evaluation of the vibrational frequencies. The values obtained often requires some sort of scaling and for several combinations of basis sets and "standard methods" like HF, MP2, B3LYP, etc…, scale factors have already been proposed. By contrast, for CASSCF, this is not possible due to the problem of the not-unique definition of the active space (and possibly because of its far less common usage). Therefore, in this work we defined our scale factor trough a simple minimum error procedure: the reproduction of the vibrational frequencies of the three most important molecules for our study: *o*-benzyne, acetylene C_2H_2, and but-1,3-diyne C_4H_2. The experimental vibrational frequencies are taken from:

J. G. Radziszewski, B. A. Hess Jr., R. Zahradnik J. Am. Chem. Soc. **1992**, *114*,52-57 for *o*-benzyne;

M. Herman *Mol. Phys.* **2007**, *105*, 2217-2241 for C_2H_2;

A. C. Simmonett, H. F. Schaefer III, W. D. Allen *J. Chem. Phys.* **2009**, *130*, Art. 044301 for C_4H_2.

***o*-Benzyne**

	exp.	CAS	scaled	error	error^2
a_1	589	634	590	1	1
	982	1012	942	-40	1627
	1039	1053	980	-59	3503
	1055	1197	1114	59	3458
	1271	1358	1264	-7	54
	1415	1554	1446	31	961
	1846	1943	1808	-38	1447
	3071	3328	3097	26	661
	3094	3361	3127	33	1116
b_1	388	419	390	2	4
	737	778	724	-13	171
	838	969	902	64	4052
b_2	472	559	520	48	2318
	849	926	862	13	160
	1094	1139	1060	-34	1167
	1307	1318	1226	-81	6497
	1394	1501	1397	3	7
	1451	1570	1461	10	98
	3049	3310	3080	31	958
	3086	3358	3125	39	1491

C_2H_2

	exp.	CAS	scaled	error	error^2
σ_g^+	3397	3649	3395	-2	3
σ_u^+	3317	3556	3309	-8	67
σ_g^+	1982	2065	1921	-60	3647
π_u	729	664	618	-111	12390
π_g	609	531	494	-114	13081

C_4H_2

	exp.	CAS	scaled	error	error^2
σ_g^+	3329	3606	3355	26	674
σ_u^+	3293	3605	3354	61	3775
σ_g^+	2184	2320	2158	-26	658
σ_u^+	2020	2126	1978	-42	1762
σ_g^+	874	910	846	-28	765
π_u	630	579	539	-91	8264
π_g	627	574	534	-93	8650
π_g	482	447	416	-66	4375
π_u	231	215	200	-31	982

Optimal scale factor: **0.9305** ***Mean error:*** ***43.9944***

Absolute (au) and Relative (kcal mol^{-1}) energies for species in Scheme 1

	CAS(12,12)/cc-pVTZ		CAS(12,12)-PT2/cc-pVTZ			CAS(12,12)-PT2/cc-pVQZ			PT2/CBS	
	E/au	*ZPE*	E/au	*Ref. W.*	E(0K)	E/au	*Ref. W.*	E(0K)	E/au	E(0K)
***o*-Benzyne**	-229.652236	0.078098	-230.403530	0.80691	***0.00***	-230.473480	0.80195	***0.00***	-230.524525	***0.00***
TS_C	-229.515802	0.067163	-230.250463	0.80858	***89.67***	-230.320331	0.80322	***89.72***	-230.371315	***89.76***
TS_1	-229.526019	0.069294	-230.260971	0.80712	***84.32***	-230.329489	0.80179	***85.22***	-230.379488	***85.87***
I_t	-229.531280	0.068633	-230.261677	0.80792	***83.49***	-230.329802	0.80269	***84.64***	-230.379515	***85.47***
TS_2	-229.521504	0.065464	-230.256660	0.80563	***84.79***	-230.325691	0.80017	***85.37***	-230.376066	***85.79***
I_c	-229.535430	0.068646	-230.264946	0.80850	***81.45***	-230.333163	0.80325	***82.53***	-230.382943	***83.33***
TS_3	-229.532492	0.067473	-230.263973	0.80782	***81.37***	-230.332423	0.80258	***82.31***	-230.382374	***83.00***
II_c	-229.541440	0.068938	-230.271475	0.80825	***77.52***	-230.339743	0.80300	***78.58***	-230.389559	***79.35***
TS_4	-229.535296	0.066010	-230.260529	0.81012	***82.68***	-230.329512	0.80475	***83.29***	-230.379851	***83.73***
C_2H_2	-76.917825	0.026564	-77.157508	0.93104	/	-77.181291	0.92868	/	-77.198646	/
C_4H_2	-152.689576	0.036895	-153.144696	0.87642	/	-153.190246	0.87249	/	-153.223485	/
Frags	-229.607401	0.063459	-230.302203	--------	***55.04***	-230.371537	--------	***55.43***	-230.422131	***55.71***
$TS_{4'}$	*-229.530629 SOSP*		-230.255021	0.80986		-230.323912	0.80446		-230.374184	
$TS_{2'}$	-229.526708	0.065746	-230.261366	0.80672	***82.00***	-230.329931	0.80141	***82.87***	-230.379965	***83.50***
II_t	-229.535396	0.068774	-230.265927	0.80782	***80.91***	-230.334032	0.80261	***82.06***	-230.383730	***82.91***
$TS_{3'}$	-229.525652	0.067500	-230.257667	0.80764	***85.35***	-230.325971	0.80242	***86.38***	-230.375814	***87.13***

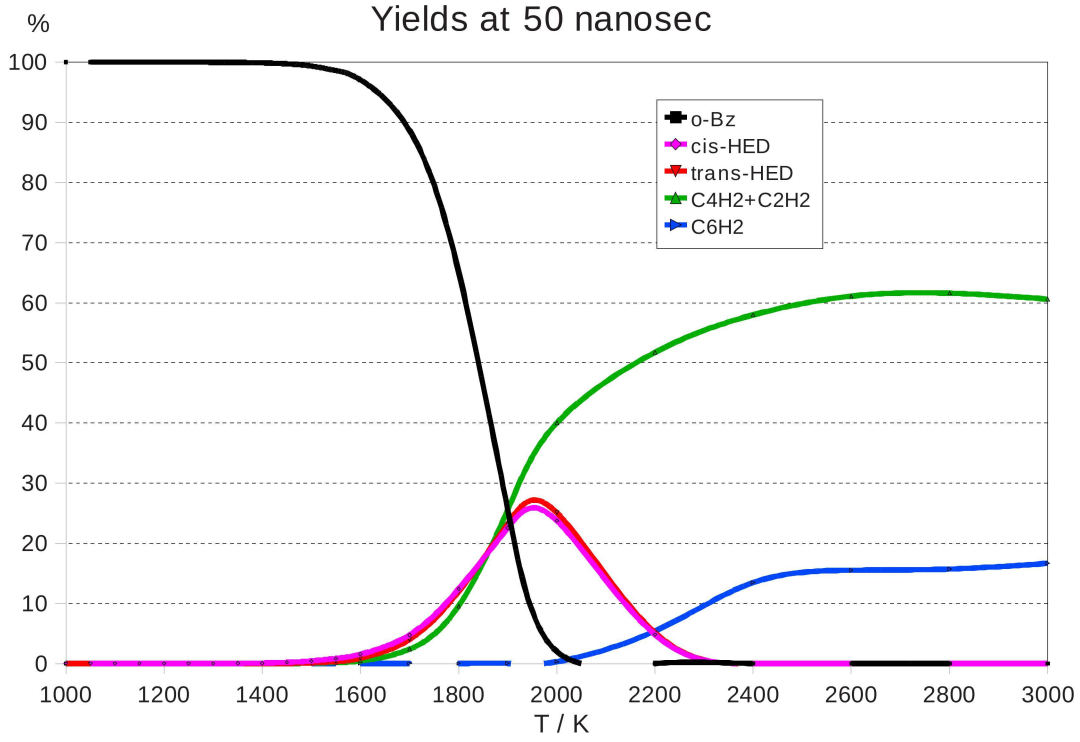
Absolute (au) and Relative (kcal mol^{-1}) energies for species in Scheme 2

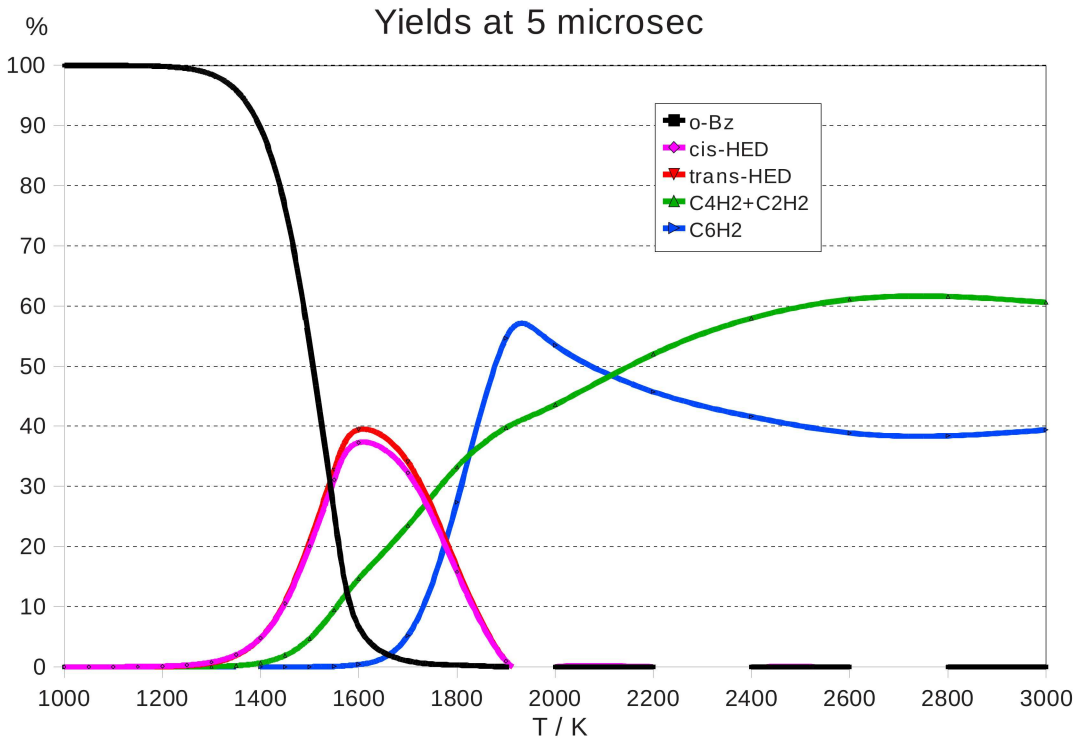
	CAS(12,12)/cc-pVTZ		CAS(12,12)-PT2/cc-pVTZ			CAS(12,12)-PT2/cc-pVQZ			PT2/CBS	
	E/au	*ZPE*	E/au	*Ref. W.*	E(0K)	E/au	*Ref. W.*	E(0K)	E/au	E(0K)
C_2H_2	-76.917825	0.026564	-77.157508	0.93104	/	-77.181291	0.92868	/	-77.198646	/
C_4H_2	-152.689576	0.036895	-153.144696	0.87642	/	-153.190246	0.87249	/	-153.223485	/
Frags	-229.607401	0.063459	-230.302203	/	**55.04**	-230.371537	/	**55.43**	-230.422131	**55.71**
TS_1	-229.515802	0.067163	-230.250463	0.80858	**89.67**	-230.320331	0.80322	**89.72**	-230.371315	**89.76**
TS_C	-229.526019	0.069294	-230.260971	0.80712	**84.32**	-230.329489	0.80179	**85.22**	-230.379488	**85.87**
o-Benzyne	-229.652427	0.078186	-230.406294	0.80588	**0.00**	-230.476234	0.80093	**0.00**	-230.527272	**0.00**
TS_{13}	-229.603222	0.075517	-230.342204	0.80585	**38.19**	-230.417655	0.80066	**34.73**	-230.472715	**32.21**
CPDene	-229.502293	0.070586	-230.351826	0.80676	**32.62**	-230.420644	0.80186	**33.33**	-230.470862	**33.84**
TS_6	-229.502293	0.070586	-230.287984	0.79644	**69.81**	-230.358292	0.79158	**69.57**	-230.409598	**69.41**
***m*-Benzyne**	-229.623149	0.077021	-230.386324	0.80032	**11.85**	-230.455879	0.79535	**12.09**	-230.506636	**12.27**
TS_7	-229.561406	0.067324	-230.295535	0.81095	**63.16**	-230.364425	0.80585	**63.82**	-230.414697	**64.30**
***cis*-HED**	-229.653025	0.071405	-230.369810	0.81753	**18.94**	-230.439396	0.81232	**19.16**	-230.490175	**19.32**
TS_8	-229.582967	0.072223	-230.327440	0.80666	**46.00**	-230.396845	0.80149	**46.34**	-230.447492	**46.58**
***p*-Benzyne**	-229.608567	0.076505	-230.361564	0.80422	**27.09**	-230.430389	0.79925	**27.79**	-230.480613	**28.30**
TS_{12}	-229.484737	0.057561	-230.199841	0.81355	**117.51**	-230.268161	0.80835	**118.53**	-230.318017	**119.27**
IV	-228.984919	0.057461	-229.699663	0.81377	/	-229.767821	0.80860	/	-229.817557	/
IV + H	-229.484729	0.057461	-230.199473	/	**117.69**	-230.267766	/	**118.72**	-230.317602	**119.48**
TS_9	-229.557872	0.065517	-230.287361	0.81049	**67.24**	-230.356256	0.80524	**67.89**	-230.406532	**68.37**
***trans*-HED**	-229.653873	0.071117	-230.370175	0.81764	**18.54**	-230.439600	0.81250	**18.86**	-230.490262	**19.10**
TS_{10}	-229.495770	0.063772	-230.236845	0.80434	**97.92**	-230.305479	0.79906	**98.74**	-230.355563	**99.34**
TS_{11}	-229.484776	0.056997	-230.199773	0.81341	**117.23**	-230.267970	0.80825	**118.32**	-230.317735	**119.12**
TS_5	-229.473666	0.064555	-230.223807	0.80159	**106.56**	-230.293493	0.79669	**106.72**	-230.344345	**106.83**
III	-228.964666	0.062356	-229.725138	0.79907	/	-229.793844	0.79413	/	-229.843981	/
III + H	-229.464476	0.062356	-230.224948	/	**104.56**	-230.293790	/	**105.25**	-230.344026	**105.75**

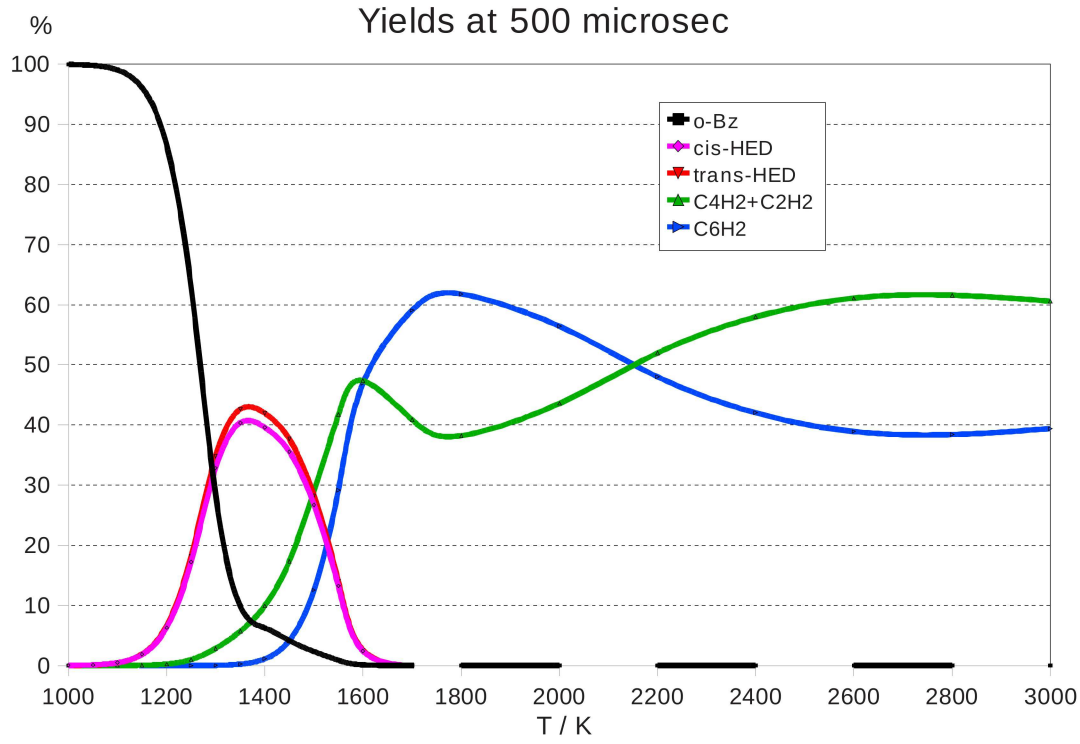
Kinetic rate constants (s-1)

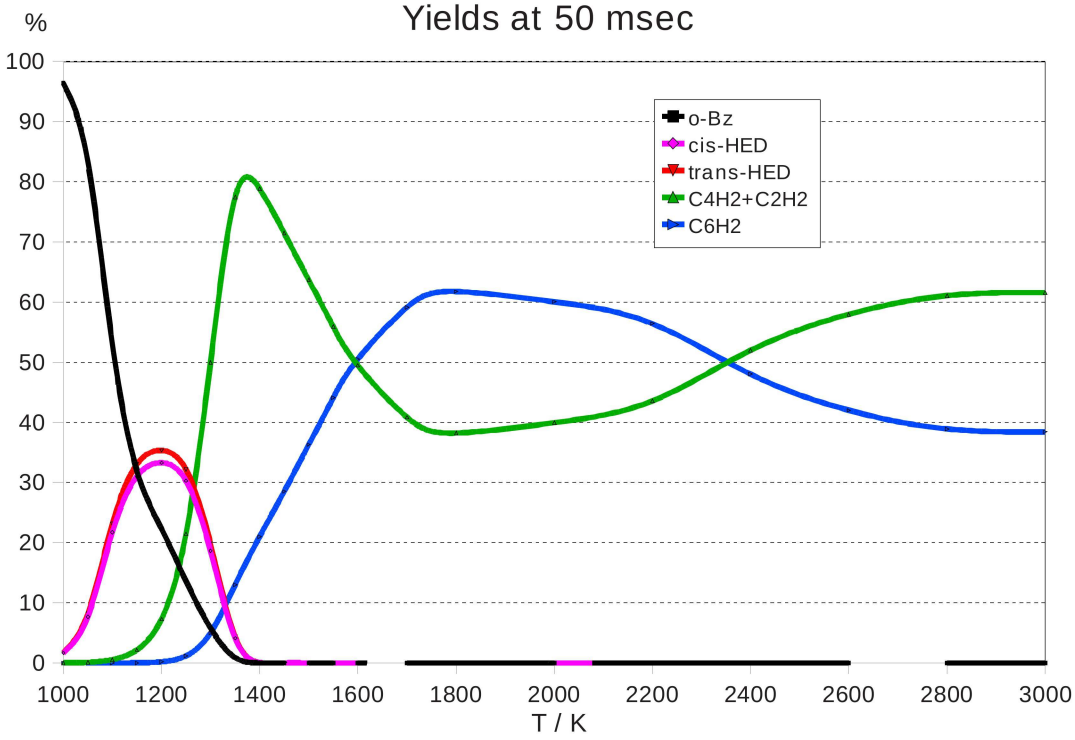
T /K	k_C	k_1	k_5	k_6	k_{-6}	k_7	k_{-7}	k_8	k_{-8}	k_9	k_{-9}	k_{10}	k_{11}	k_{12}
600	9.1E-19	1.4E-16	1.3E-22	3.3E-11	9.3E-08	2.3E-04	7.9E-04	2.7E+01	1.2E+07	7.0E-05	6.4E-05	7.9E-17	2.4E-21	1.2E-20
800	3.5E-10	1.8E-08	1.5E-12	9.2E-05	1.9E-02	2.8E+01	1.1E+01	6.4E+03	8.3E+08	3.0E+00	2.8E+00	2.0E-09	3.4E-12	3.2E-11
850	1.1E-08	4.8E-07	8.7E-11	1.3E-03	1.6E-01	2.2E+02	6.1E+01	1.7E+04	1.8E+09	2.0E+01	1.9E+01	4.0E-08	1.4E-10	1.5E-09
900	2.4E-07	9.2E-06	3.3E-09	1.3E-02	1.1E+00	1.4E+03	2.8E+02	4.0E+04	3.4E+09	1.1E+02	9.9E+01	5.8E-07	3.7E-09	4.6E-08
950	3.8E-06	1.3E-04	8.8E-08	1.1E-01	6.2E+00	7.2E+03	1.1E+03	8.5E+04	6.2E+09	4.8E+02	4.5E+02	6.4E-06	7.0E-08	9.9E-07
1000	4.6E-05	1.4E-03	1.7E-06	6.9E-01	2.9E+01	3.2E+04	3.6E+03	1.7E+05	1.1E+10	1.9E+03	1.8E+03	5.6E-05	9.7E-07	1.6E-05
1025	1.5E-04	4.2E-03	6.5E-06	1.7E+00	6.0E+01	6.4E+04	6.3E+03	2.4E+05	1.4E+10	3.5E+03	3.3E+03	1.5E-04	3.3E-06	5.6E-05
1050	4.4E-04	1.2E-02	2.4E-05	3.8E+00	1.2E+02	1.2E+05	1.1E+04	3.2E+05	1.7E+10	6.4E+03	6.0E+03	4.0E-04	1.1E-05	1.9E-04
1100	3.4E-03	8.4E-02	2.7E-04	1.8E+01	4.2E+02	4.2E+05	2.9E+04	5.6E+05	2.7E+10	2.0E+04	1.8E+04	2.4E-03	9.1E-05	1.9E-03
1150	2.2E-02	5.0E-01	2.5E-03	7.3E+01	1.3E+03	1.3E+06	7.3E+04	9.4E+05	4.1E+10	5.4E+04	5.1E+04	1.2E-02	6.5E-04	1.5E-02
1200	1.2E-01	2.6E+00	1.9E-02	2.7E+02	3.9E+03	3.6E+06	1.7E+05	1.5E+06	5.9E+10	1.4E+05	1.3E+05	5.4E-02	3.9E-03	1.0E-01
1250	5.9E-01	1.2E+01	1.2E-01	8.8E+02	1.0E+04	9.3E+06	3.6E+05	2.4E+06	8.4E+10	3.3E+05	3.1E+05	2.1E-01	2.0E-02	5.9E-01
1300	2.5E+00	4.7E+01	7.0E-01	2.7E+03	2.6E+04	2.2E+07	7.4E+05	3.5E+06	1.2E+11	7.3E+05	6.9E+05	7.6E-01	9.3E-02	3.0E+00
1350	9.7E+00	1.7E+02	3.5E+00	7.4E+03	5.9E+04	5.0E+07	1.4E+06	5.1E+06	1.6E+11	1.5E+06	1.4E+06	2.5E+00	3.8E-01	1.4E+01
1400	3.4E+01	5.7E+02	1.5E+01	1.9E+04	1.3E+05	1.1E+08	2.6E+06	7.3E+06	2.0E+11	3.0E+06	2.9E+06	7.4E+00	1.4E+00	5.5E+01
1450	1.1E+02	1.7E+03	6.2E+01	4.6E+04	2.7E+05	2.2E+08	4.7E+06	1.0E+07	2.6E+11	5.7E+06	5.4E+06	2.0E+01	4.6E+00	2.0E+02
1500	3.3E+02	5.0E+03	2.3E+02	1.0E+05	5.3E+05	4.2E+08	8.0E+06	1.4E+07	3.3E+11	1.0E+07	9.8E+06	5.3E+01	1.4E+01	6.8E+02
1550	9.2E+02	1.3E+04	7.6E+02	2.3E+05	9.9E+05	7.7E+08	1.3E+07	1.8E+07	4.2E+11	1.8E+07	1.7E+07	1.3E+02	4.1E+01	2.1E+03
1600	2.4E+03	3.3E+04	2.4E+03	4.6E+05	1.8E+06	1.4E+09	2.1E+07	2.4E+07	5.1E+11	3.1E+07	2.9E+07	3.0E+02	1.1E+02	6.2E+03
1700	1.4E+04	1.8E+05	1.9E+04	1.7E+06	5.3E+06	3.9E+09	4.9E+07	3.8E+07	7.5E+11	8.0E+07	7.6E+07	1.4E+03	6.5E+02	4.4E+04
1800	6.7E+04	7.7E+05	1.2E+05	5.6E+06	1.4E+07	9.9E+09	1.1E+08	5.9E+07	1.1E+12	1.9E+08	1.8E+08	5.3E+03	3.2E+03	2.5E+05
1900	2.7E+05	2.9E+06	6.3E+05	1.6E+07	3.3E+07	2.3E+10	2.1E+08	8.7E+07	1.4E+12	4.0E+08	3.8E+08	1.8E+04	1.3E+04	1.2E+06
2000	9.7E+05	9.7E+06	2.8E+06	4.1E+07	7.1E+07	4.9E+10	3.9E+08	1.2E+08	1.9E+12	8.0E+08	7.6E+08	5.4E+04	4.5E+04	4.8E+06
2200	8.7E+06	7.6E+07	3.7E+07	2.1E+08	2.7E+08	1.8E+11	1.1E+09	2.3E+08	3.0E+12	2.6E+09	2.5E+09	3.6E+05	3.9E+05	5.5E+07
2400	5.4E+07	4.3E+08	3.2E+08	8.1E+08	8.2E+08	5.3E+11	2.7E+09	3.7E+08	4.5E+12	7.0E+09	6.7E+09	1.7E+06	2.3E+06	4.1E+08
2600	2.6E+08	1.9E+09	2.0E+09	2.6E+09	2.1E+09	1.3E+12	5.7E+09	5.7E+08	6.2E+12	1.6E+10	1.5E+10	6.6E+06	1.0E+07	2.3E+09
2800	9.9E+08	6.5E+09	9.4E+09	6.9E+09	4.7E+09	2.9E+12	1.1E+10	8.2E+08	8.3E+12	3.3E+10	3.2E+10	2.1E+07	3.7E+07	1.0E+10
3000	3.2E+09	1.9E+10	3.7E+10	1.6E+10	9.6E+09	5.8E+12	1.9E+10	1.1E+09	1.1E+13	6.2E+10	5.9E+10	5.7E+07	1.1E+08	3.6E+10
3200	8.9E+09	5.0E+10	1.2E+11	3.4E+10	1.8E+10	1.1E+13	3.1E+10	1.5E+09	1.3E+13	1.1E+11	1.0E+11	1.4E+08	2.8E+08	1.1E+11
3400	2.2E+10	1.2E+11	3.4E+11	6.6E+10	3.0E+10	1.8E+13	4.8E+10	1.9E+09	1.6E+13	1.7E+11	1.7E+11	2.9E+08	6.5E+08	2.9E+11

Product yields as funcion of temperature and elapsed time.




Yields at 5 microsec
%
100
90
80
70
60
50
40
30
20
10
0
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
T / K
o-Bz
cis-HED
trans-HED
C4H2+C2H2
C6H2


Yields at 500 microsec
%
100
90
80
70
60
50
40
30
20
10
0
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
T / K
o-Bz
cis-HED
trans-HED
C4H2+C2H2
C6H2


Yields at 50 msec
%
100
90
80
70
60
50
40
30
20
10
0
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
T / K
o-Bz
cis-HED
trans-HED
C4H2+C2H2
C6H2

Geometries CAS(12,12)-PT2(FC)/cc-pVTZ
(Symmetry and Cartesian coordinates Angstrom):
Active Molecular Orbitals Occupations
Vibrational frequencies

C2H2 (C_{2v})

No.	Label	X	Y	Z
1	C2	0.00000	0.00000	0.60392
2	H4	0.00000	0.00000	1.66418
3	C2	0.00000	0.00000	-0.60392
4	H4	0.00000	0.00000	-1.66418

Natural orbitals and occupation numbers for root 1
sym 2: 1.937971 1.937971
sym 4: 0.062029 0.062029

Vibrational frequencies (cm-1)
531.28
531.28
663.91
663.91
2064.92
3555.83
3648.99

C4H2 (C_{2v})

No.	Label	X	Y	Z
1	C2	0.00000	0.00000	0.68594
2	C4	0.00000	0.00000	1.89948
3	H5	0.00000	0.00000	2.96001
4	C2	0.00000	0.00000	-0.68594
5	C4	0.00000	0.00000	-1.89948
6	H5	0.00000	0.00000	-2.96001

Natural orbitals and occupation numbers for root 1
sym 2: 1.948503 1.948503 0.085578 0.085579
sym 4: 1.921878 1.921878 0.044040 0.044040

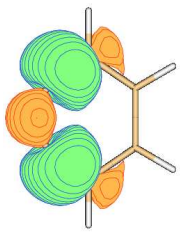
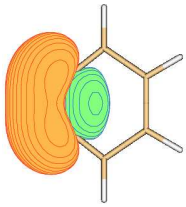
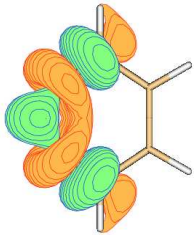
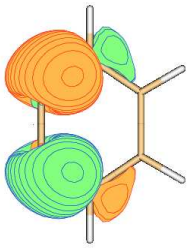
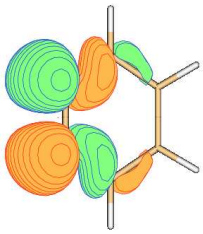
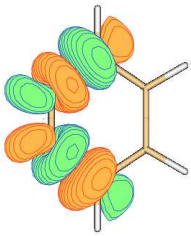
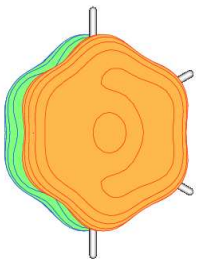
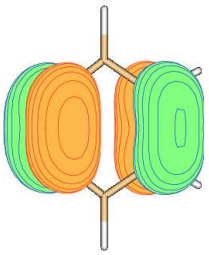
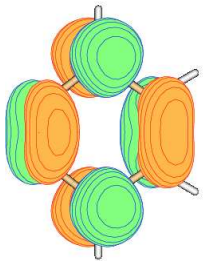
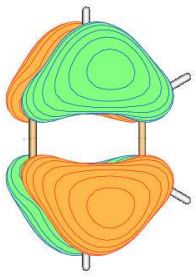
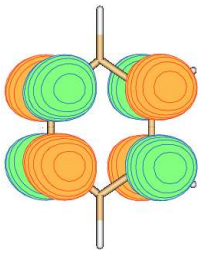
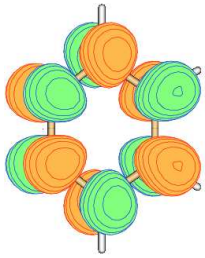
Vibrational frequencies (cm-1)
214.57
214.60
446.92
446.92
573.88
573.88
579.36
579.37
909.56

```
  2125.77
  2319.56
  3604.99
  3605.54
 -------------------------------
```

***ortho*-Benzyne (C_{2v})**

```
 ----------------------------------------
No.  Label     X         Y         Z
 ----------------------------------------
 1   C3       0.63145   0.00000   0.19381
 2   C4       1.45557   0.00000   1.30326
 3   C5       0.70132   0.00000   2.49520
 4   H6       2.53340   0.00000   1.30009
 5   H7       1.22306   0.00000   3.44150
 6   C3      -0.63145   0.00000   0.19381
 7   C4      -1.45557   0.00000   1.30326
 8   C5      -0.70132   0.00000   2.49520
 9   H6      -2.53340   0.00000   1.30009
10   H7      -1.22306   0.00000   3.44150
 ----------------------------------------

 Natural orbitals and occupation numbers for root  1
```

1.978	1.837	0.020	1.979	0.171	0.014
					
1.958	**1.909**	**0.099**	**1.904**	**0.091**	**0.039**
					

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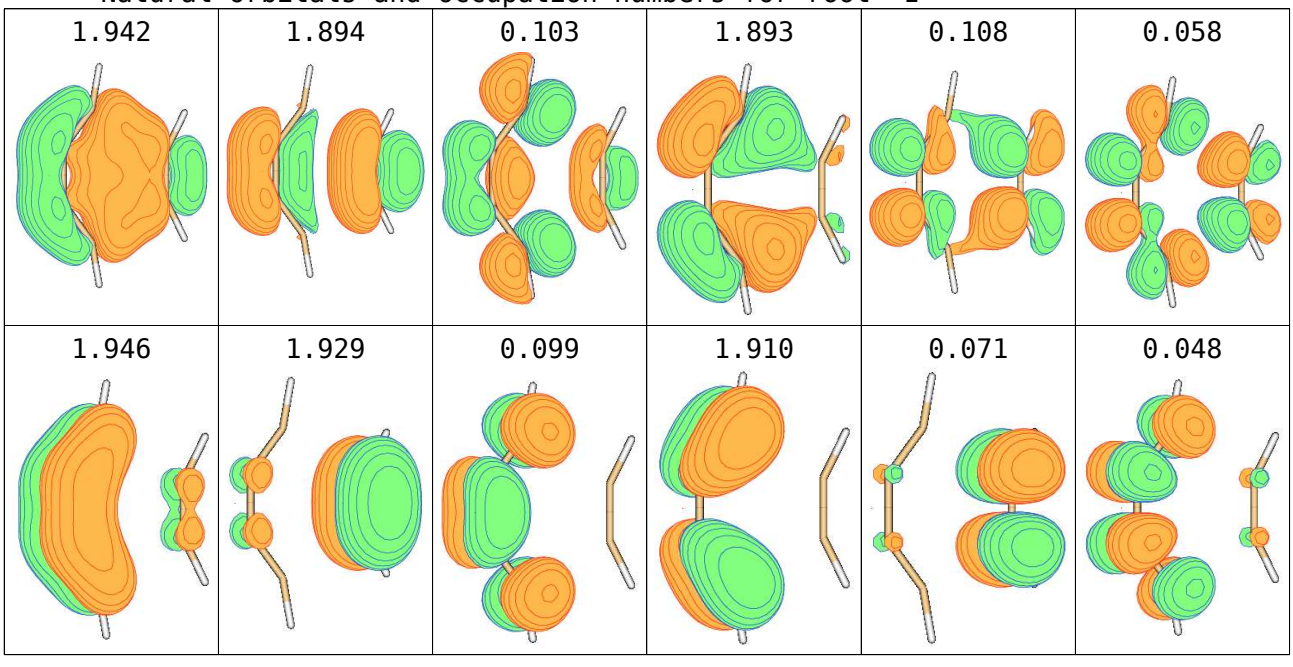
 -------------------------------
 Vibrational frequencies (cm-1)
   418.60
   454.86
   558.54
   633.99
   635.60
   777.58
   890.21
   926.36
   968.92
  1012.18
  1014.15
  1053.34
```

```
  1139.11
  1196.82
  1318.39
  1358.24
  1501.02
  1554.02
  1569.74
  1943.26
  3309.70
  3328.08
  3358.01
  3360.55
 -------------------------------
```

TSc (C_{2v})

```
 ----------------------------------------
No.  Label     X         Y         Z
 ----------------------------------------
 1   C3       0.66859   0.00000   0.36898
 2   C4       1.65730   0.00000   1.13180
 3   C5       0.62145   0.00000   3.10572
 4   H6       2.70501   0.00000   1.32783
 5   H7       1.56405   0.00000   3.59952
 6   C3      -0.66859   0.00000   0.36898
 7   C4      -1.65730   0.00000   1.13180
 8   C5      -0.62145   0.00000   3.10572
 9   H6      -2.70501   0.00000   1.32783
10   H7      -1.56405   0.00000   3.59952
 ----------------------------------------
```

Natural orbitals and occupation numbers for root 1

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Vibrational frequencies (cm-1)
 i 833.70
    75.92
   241.49
```
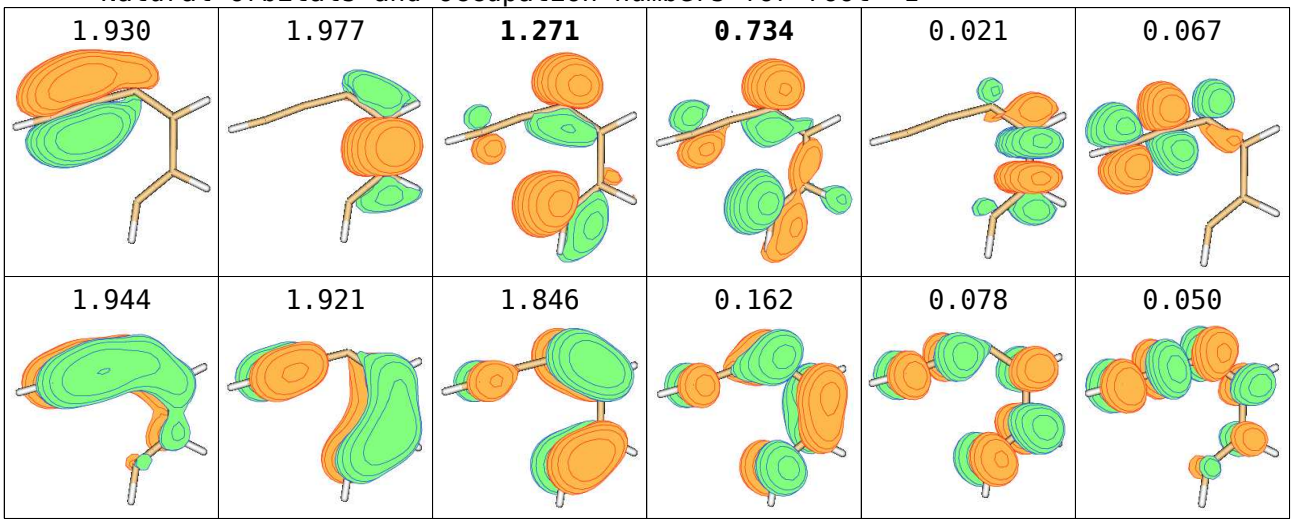

```
   298.40
   444.36
   486.54
   509.73
   552.64
   623.83
   635.60
   652.00
   661.53
   730.75
   905.70
   940.44
   942.42
  1158.19
  1716.49
  1857.90
  2014.57
  3483.58
  3507.05
  3507.79
  3534.10
 ------------------------------
```

TS_1 (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.22817
3	C3	0.12287	0.00000	2.57252
4	C4	1.16315	0.00000	3.40169
5	C5	2.56533	0.00000	2.89363
6	C6	2.99134	0.00000	1.64578
7	H7	1.04128	0.00000	4.47359
8	H8	-0.08120	0.00000	-1.05766
9	H9	3.30921	0.00000	3.68463
10	H10	3.93941	0.00000	1.14134

Natural orbitals and occupation numbers for root 1



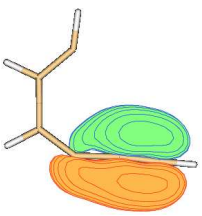
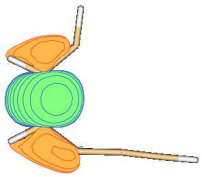
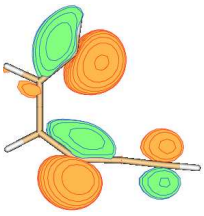
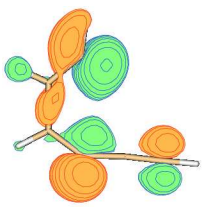
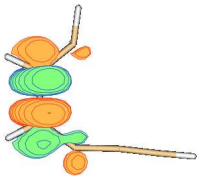
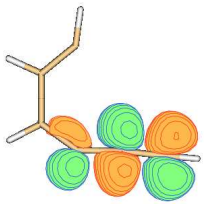
Vibrational frequencies (cm-1)

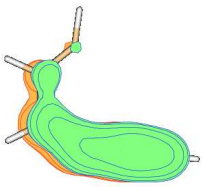
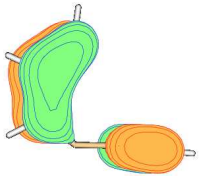
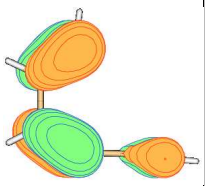
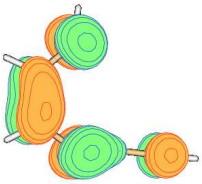
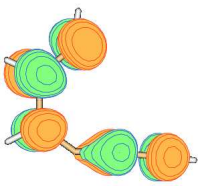
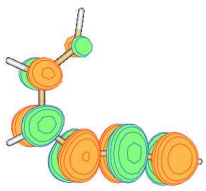
i	195.90
	209.66
	287.02
	354.21
	471.30
	490.80
	537.87
	611.33
	614.71
	702.68
	766.48
	849.01
	853.17
	985.98
	1042.96
	1316.65
	1355.86
	1541.99
	1714.24
	2007.43
	3313.57
	3370.17
	3413.61
	3600.19

I_t (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.34368
3	C4	-0.09760	0.00000	-1.22700
4	H5	-0.18097	0.00000	-2.28439
5	C6	0.73981	0.00000	2.44823
6	H7	0.24649	0.00000	3.40987
7	C8	2.21788	0.00000	2.48363
8	C9	3.05339	0.00000	1.45714
9	H10	2.64163	0.00000	3.48397
10	H11	4.12068	0.00000	1.33100

Natural orbitals and occupation numbers for root 1

1.929	1.979	**1.121**	**0.883**	0.020	0.068
					

1.944	1.920	1.838	0.171	0.080	0.049
					

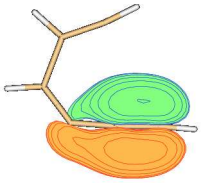
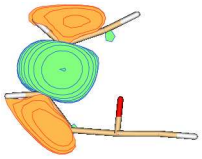
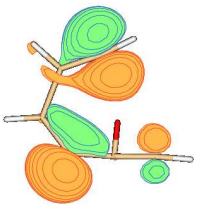
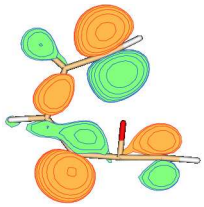
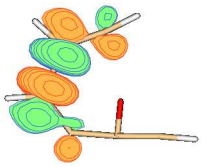
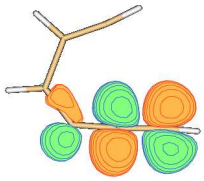
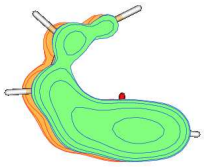
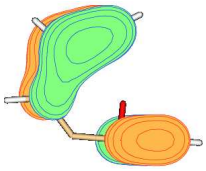
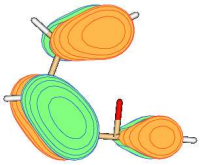
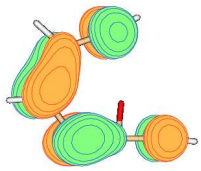
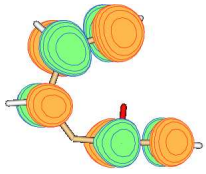
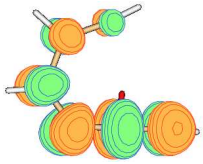
Vibrational frequencies (cm-1)

93.35
102.24
260.81
290.15
441.48
485.90
499.80
521.84
617.53
691.88
774.71
829.12
858.38
909.48
1054.86
1362.04
1393.12
1559.95
1729.17
2063.84
3273.09
3319.59
3391.39
3602.53

TS_2 (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.35344
3	X3	0.99956	0.00000	-0.02983
4	C4	0.08303	0.00000	-1.22495
5	H5	0.08174	0.00000	-2.28690
6	C6	0.99147	0.00000	2.22768
7	H7	0.84795	0.00000	3.29707
8	C8	2.45837	0.00000	1.78375
9	C9	2.95906	0.00000	0.58468
10	H10	3.11308	0.00000	2.65071
11	H11	3.48753	0.00000	-0.33582

Natural orbitals and occupation numbers for root 1

1.931	1.973	**1.418**	**0.588**	0.024	0.065
					
1.945	1.924	1.867	0.142	0.074	0.049
					

sym 1: 1.931251 1.972704 1.419585 0.585991 0.024174 0.065238
sym 2: 1.944987 1.924346 1.866884 0.141604 0.074118 0.049116

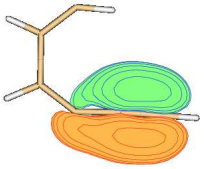
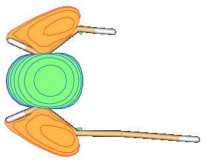
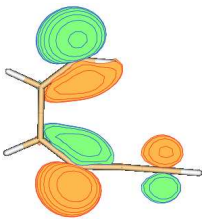
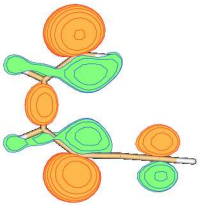
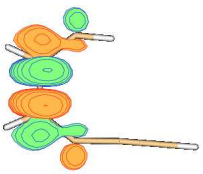
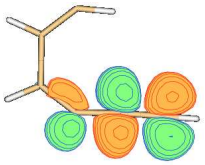
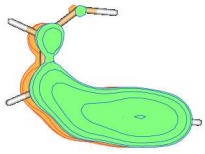
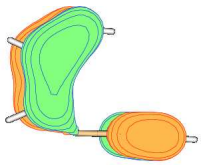
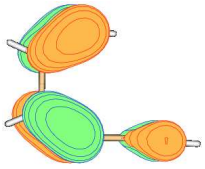
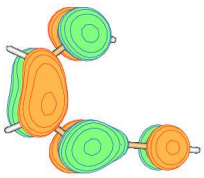
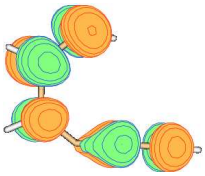
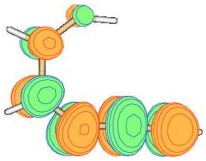
Vibrational frequencies (cm-1)

i 876.25
76.31
84.46
246.32
288.61
304.64
451.90
492.53
525.44
527.90
682.17
712.24
749.80
837.14
919.90
1259.94
1365.94
1555.07
1749.33
2097.22
3277.52
3341.58
3585.75
3603.43

I_c (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.34893
3	C4	-0.06694	0.00000	-1.22679
4	H5	-0.12672	0.00000	-2.28559
5	C6	0.78265	0.00000	2.41305

```
 6   H7       0.34954   0.00000   3.40262
 7   C8       2.29044   0.00000   2.40488
 8   C9       3.09606   0.00000   1.36427
 9   H10      2.71507   0.00000   3.40013
10   H11      3.01631   0.00000   0.29076
----------------------------------------

Natural orbitals and occupation numbers for root  1
```

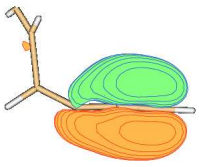
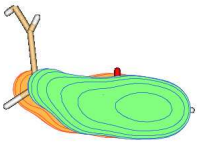
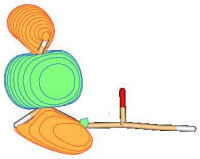
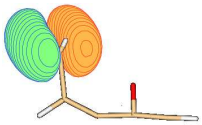
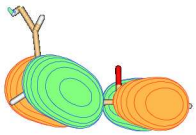
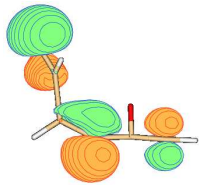
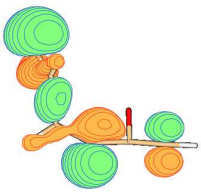
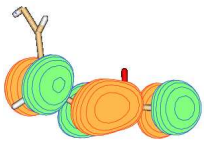
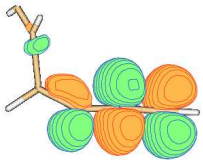
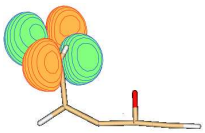
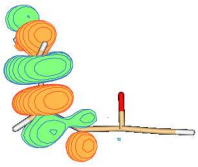
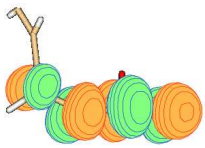
1.931	1.974	**1.259**	**0.745**	0.022	0.067
					
1.947	1.921	1.850	0.158	0.078	0.049
					

```
sym 1:   1.930862   1.974307   1.259546   0.745196   0.066503   0.022496
sym 2:   1.944604   1.920930   1.850377   0.158034   0.078281   0.048864

-------------------------------
Vibrational frequencies (cm-1)
    87.39
    97.91
   249.95
   289.67
   430.55
   486.81
   512.43
   525.55
   650.11
   694.10
   769.84
   801.28
   903.22
   923.48
  1031.45
  1304.54
  1370.31
  1552.24
  1737.02
  2082.97
  3308.63
  3332.72
  3388.19
  3601.54
-------------------------------
```

TS_3 (C_1)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.35117
3	X3	1.00000	0.00000	0.00190
4	C4	-0.12092	-0.01379	-1.22105
5	H5	-0.18146	-0.01662	-2.27993
6	C6	0.59612	0.09321	2.50512
7	H7	0.07402	0.08972	3.45186
8	C8	2.15270	0.11640	2.64017
9	C9	2.83899	1.21840	2.57859
10	H10	2.57897	-0.85401	2.85784
11	H11	2.67967	2.25641	2.34664

Natural orbitals and occupation numbers for root 1

1.933	1.944	1.970	1.915	1.899	**1.417**
					
0.589	0.108	0.065	0.086	0.025	0.048
					

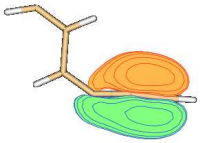
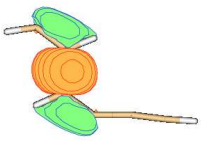
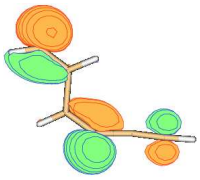
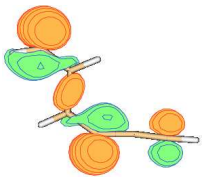
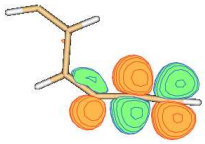
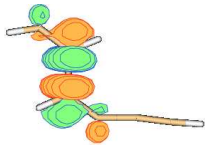
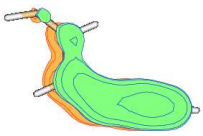
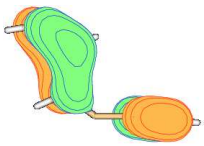
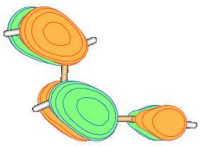
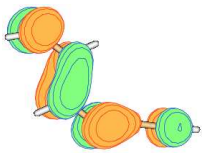
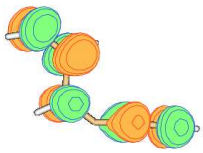
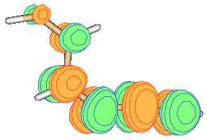
Vibrational frequencies (cm-1)
i 77.95
106.33
223.60
308.01
384.78
491.12
499.35
545.84
557.10
621.27
694.59
749.53
870.97
900.87
968.90
1203.43
1318.15
1607.77
1771.82
2121.68
3327.32

3341.70
3395.78
3607.10

II_c (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.35273
3	C4	-0.14084	0.00000	-1.21972
4	H5	-0.21072	0.00000	-2.27754
5	C6	0.74591	0.00000	2.44382
6	H7	0.31730	0.00000	3.43238
7	C8	2.24820	0.00000	2.34157
8	C9	3.01362	0.00000	3.41246
9	H10	2.64941	0.00000	1.33909
10	H11	2.86234	0.00000	4.47820

Natural orbitals and occupation numbers for root 1

1.931	1.974	**1.337**	**0.667**	0.067	0.022
					
1.942	1.924	1.855	0.153	0.076	0.048
					

Vibrational frequencies (cm-1)

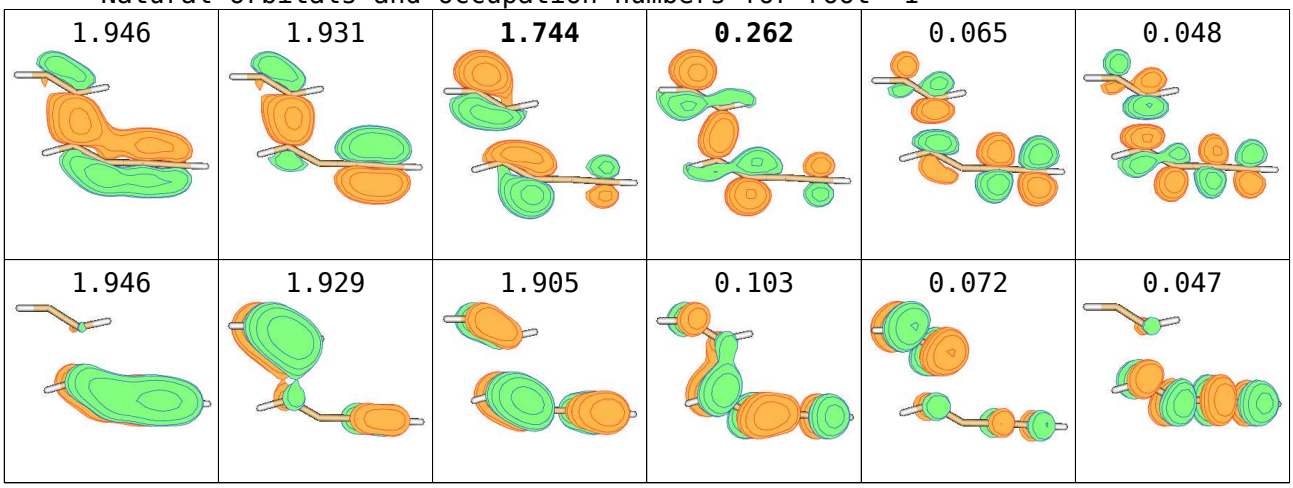
104.84
117.85
253.51
334.11
386.53
482.46
510.15
525.56
628.33
660.09
823.97
825.88
909.42
916.22
1013.60
1332.47
1378.54
1580.56

1712.95
2092.64
3336.28
3353.77
3378.12
3602.56

TS_4 (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.36154
3	C4	-0.06633	0.00000	-1.21890
4	H5	-0.09700	0.00000	-2.27883
5	C6	0.58663	0.00000	2.48636
6	H7	0.30072	0.00000	3.51642
7	C8	2.44147	0.00000	2.39294
8	C9	3.07402	0.00000	3.48414
9	H10	2.66817	0.00000	1.34557
10	H11	3.06391	0.00000	4.55234

Natural orbitals and occupation numbers for root 1



Vibrational frequencies (cm-1)

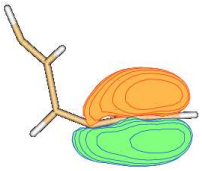
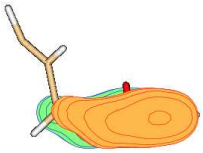
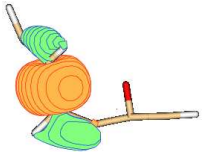
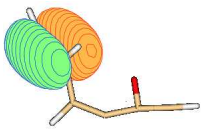
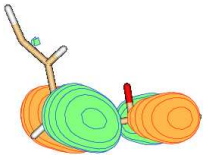
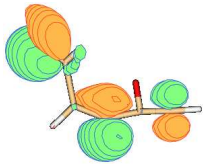
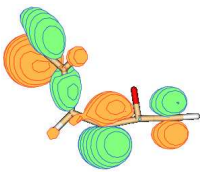
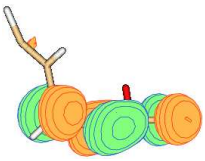
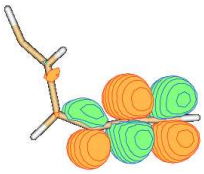
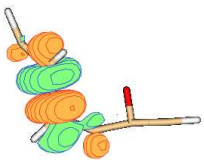
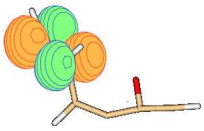
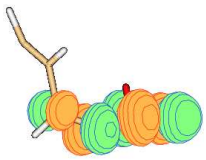
i 762.07
57.62
89.87
241.47
322.81
346.79
482.33
525.69
548.77
560.71
612.41
720.52
813.05
838.31
910.09

1133.90
1177.03
1663.32
1835.08
2162.20
3420.16
3450.89
3457.33
3604.73

$TS_{3'}$ (C_1)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.34870
3	X3	1.00000	0.00000	0.00000
4	C4	-0.18959	0.00000	-1.21534
5	H5	-0.31453	-0.01276	-2.26995
6	C6	0.63677	0.02567	2.49746
7	H7	0.10229	0.01315	3.43816
8	C8	2.15624	-0.00086	2.59258
9	C9	2.87928	1.07291	2.75387
10	H10	2.59447	-0.99420	2.54531
11	H11	3.90327	1.36102	2.90263

Natural orbitals and occupation numbers for root 1

1.931	1.943	1.977	1.912	1.893	**1.265**
					
0.740	0.115	0.067	0.021	0.089	0.050
					

Vibrational frequencies (cm-1)
i 121.27
103.69
215.80
313.92
389.36
466.67
476.10
522.16
532.46
665.18

716.44
733.75
811.30
906.95
1020.24
1292.61
1326.87
1622.12
1760.77
2100.39
3299.72
3340.86
3420.15
3620.65

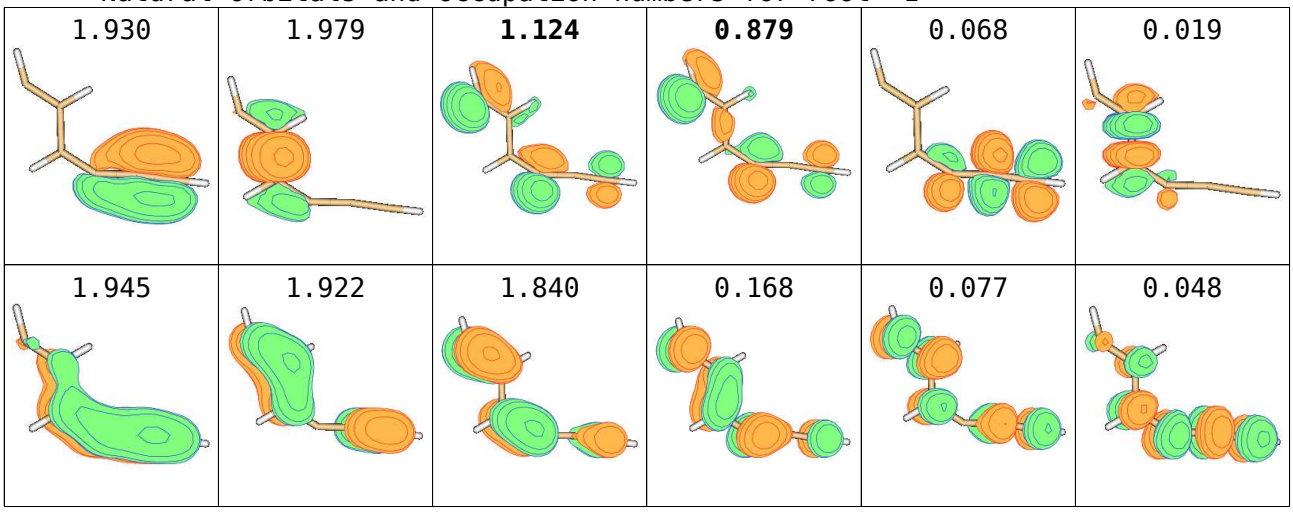
8

II_t (C_s)

Cartesian coordinates in Angstrom:

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.34177
3	C4	-0.14110	0.00000	-1.22399
4	H5	-0.23239	0.00000	-2.27997
5	C6	0.66840	0.00000	2.49119
6	H7	0.12662	0.00000	3.42616
7	C8	2.13661	0.00000	2.56890
8	C9	2.80283	0.00000	3.71129
9	H10	2.67133	0.00000	1.62397
10	H11	3.83072	0.00000	4.02511

Natural orbitals and occupation numbers for root 1



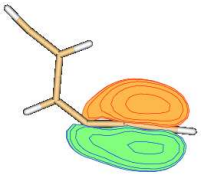
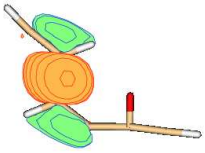
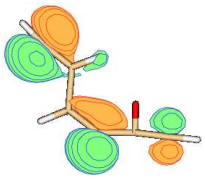
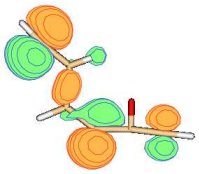
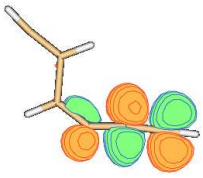
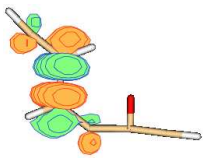
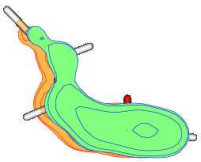
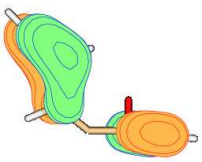
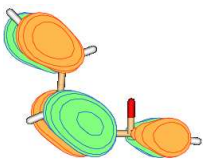
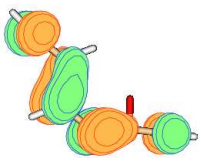
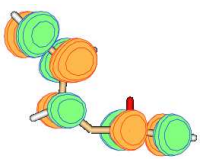
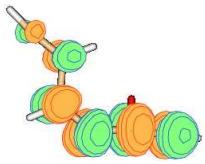
Vibrational frequencies (cm-1)
104.84
117.85
253.51
334.11

```
  386.53
  482.46
  510.15
  525.56
  628.33
  660.09
  823.97
  825.88
  909.42
  916.22
 1013.60
 1332.47
 1378.54
 1580.56
 1712.95
 2092.64
 3336.28
 3353.77
 3378.12
 3602.56
-------------------------------
```

$TS_{2'}$

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.35330
3	X3	0.99995	0.00000	-0.00973
4	C4	-0.13539	0.00000	-1.22078
5	H5	-0.22827	0.00000	-2.27681
6	C6	0.77472	0.00000	2.42729
7	H7	0.36559	0.00000	3.42412
8	C8	2.28166	0.00000	2.31134
9	C9	3.05863	0.00000	3.35712
10	H10	2.65204	0.00000	1.29127
11	H11	3.80056	0.00000	4.11970

Natural orbitals and occupation numbers for root 1

1.931	1.975	**1.316**	**0.689**	0.067	0.022
					
1.945	1.926	1.862	0.146	0.073	0.048
					

Vibrational frequencies (cm-1)

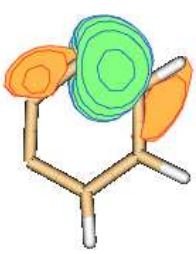
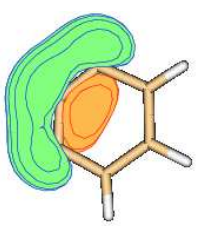
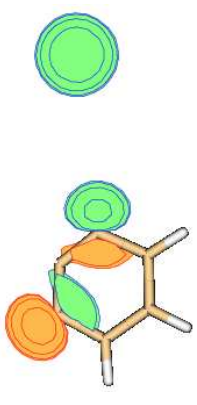
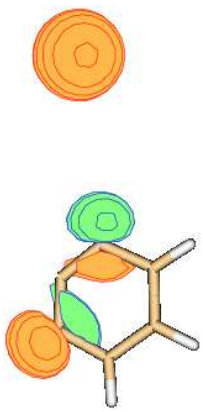
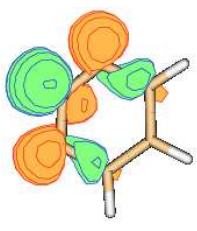
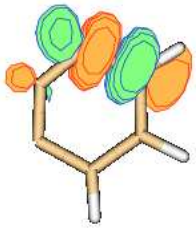
i	869.57
	100.83
	337.71
	413.16
	511.11
	625.91
	771.05
	907.58
	1312.04
	1370.30
	1572.39
	1724.45
	2097.95
	3295.82
	3367.20
	3581.38
	3603.24
	112.74
	246.66
	279.11
	487.76
	525.69
	779.13
	836.17

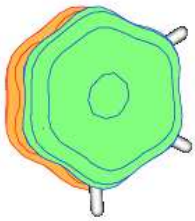
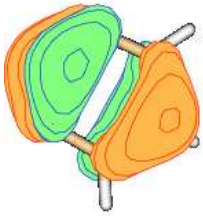
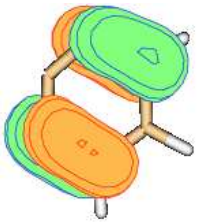
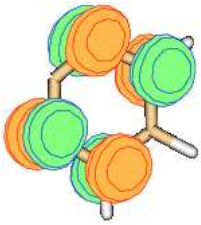
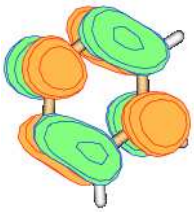
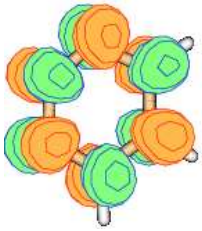
TS_5 (C_s)

Cartesian coordinates in Angstrom:

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.30338
3	C3	0.98184	0.00000	2.14317
4	C4	2.28276	0.00000	1.62395
5	C5	2.37511	0.00000	0.22110
6	C6	1.24880	0.00000	-0.62663
7	H7	3.16936	0.00000	2.23854
8	H8	3.35903	0.00000	-0.23035
9	H9	1.36799	0.00000	-1.69913
10	H10	0.22868	0.00000	6.75512

Natural orbitals and occupation numbers for root 1

1.978	1.801	**1.019**	**0.984**	0.201	0.018
					

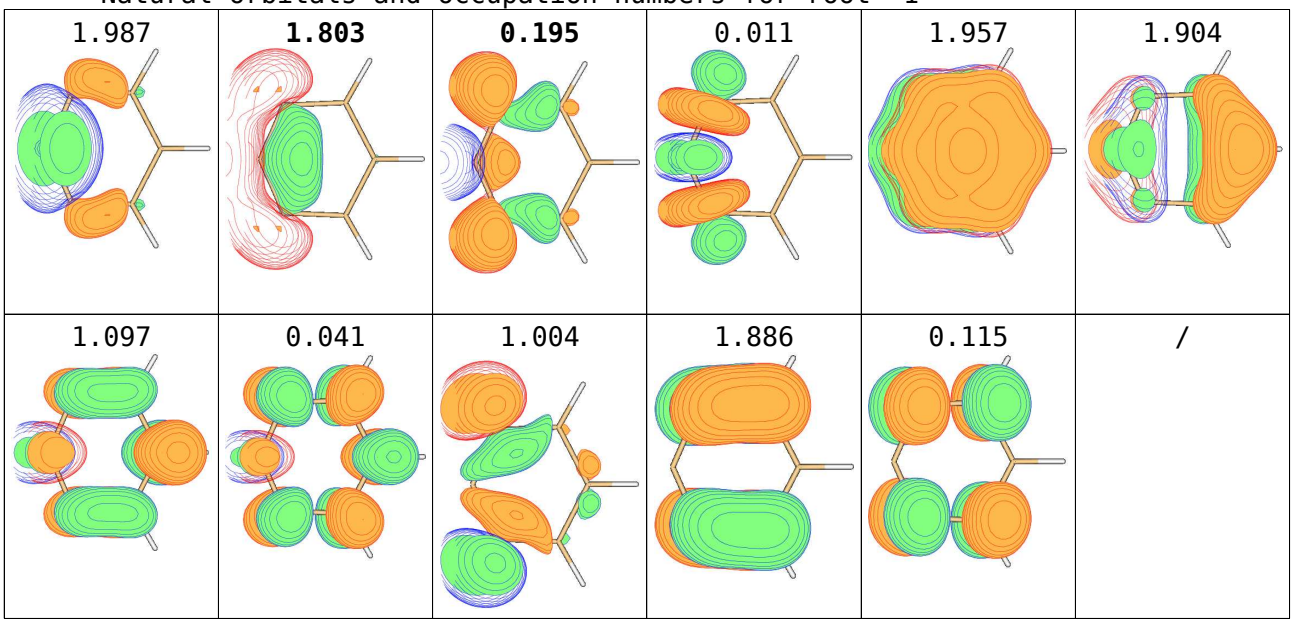
1.957	1.906	1.891	0.110	0.096	0.040
					

```
--------------------------------
Vibrational frequencies (cm-1)
  i 75.36
    23.27
    24.34
   410.79
   438.98
   446.02
   604.61
   634.23
   782.71
   906.63
   912.84
   990.77
  1024.15
  1091.24
  1153.81
  1193.96
  1313.63
  1423.67
  1538.34
  1576.58
  1825.39
  3315.68
  3339.12
  3365.45
--------------------------------
```

III (C_{2v})

```
----------------------------------------
No.  Label     X          Y          Z
----------------------------------------
 1   C1       0.00000    0.00000    0.00000
 2   H2       0.00000    0.00000    1.08177
 3   C4       0.00000   -1.23797   -0.67060
 4   C5       0.00000   -1.18344   -2.06830
 5   C6       0.00000    0.00000   -2.60281
 6   H7       0.00000   -2.16475   -0.11773
 7   C4       0.00000    1.23797   -0.67060
 8   C5       0.00000    1.18344   -2.06830
 9   H7       0.00000    2.16475   -0.11773
----------------------------------------
```

Natural orbitals and occupation numbers for root 1



Vibrational frequencies (cm-1)

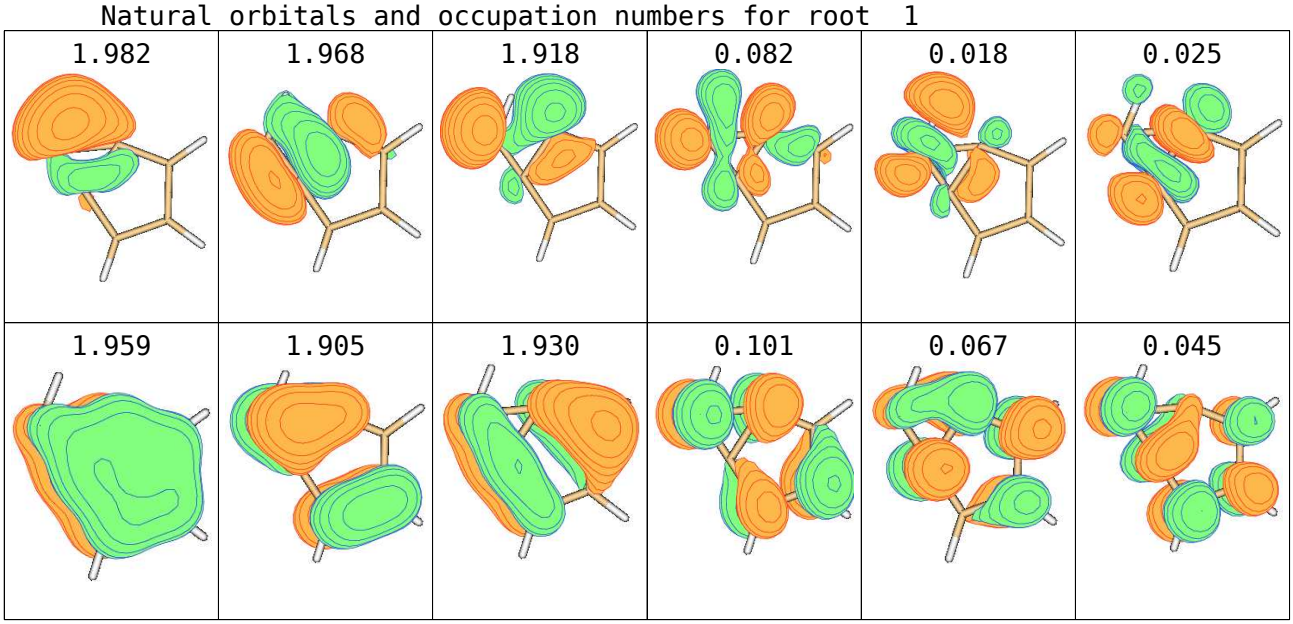
444.32
450.62
475.96
611.65
618.46
789.61
864.69
909.69
938.44
989.24
1058.76
1150.82
1180.47
1237.17
1406.04
1507.49
1563.29
1615.22
3313.73
3347.69
3353.10

TS_6 (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.62956
3	C3	0.59620	0.00000	2.87614
4	C4	2.01800	0.00000	2.70561
5	C5	2.36104	0.00000	1.35375
6	C6	1.14120	0.00000	0.67196
7	H7	-1.02525	0.00000	0.54309

8	H8	0.07217	0.00000	3.81799
9	H9	2.73316	0.00000	3.51933
10	H10	3.34661	0.00000	0.92205

Natural orbitals and occupation numbers for root 1



Vibrational frequencies (cm-1)

i 1199.65
221.02
385.52
542.00
575.46
575.60
642.87
770.54
839.32
843.40
897.82
974.60
1011.28
1065.00
1174.35
1353.07
1443.61
1476.23
1607.00
1847.41
2652.69
3326.75
3365.34
3392.69

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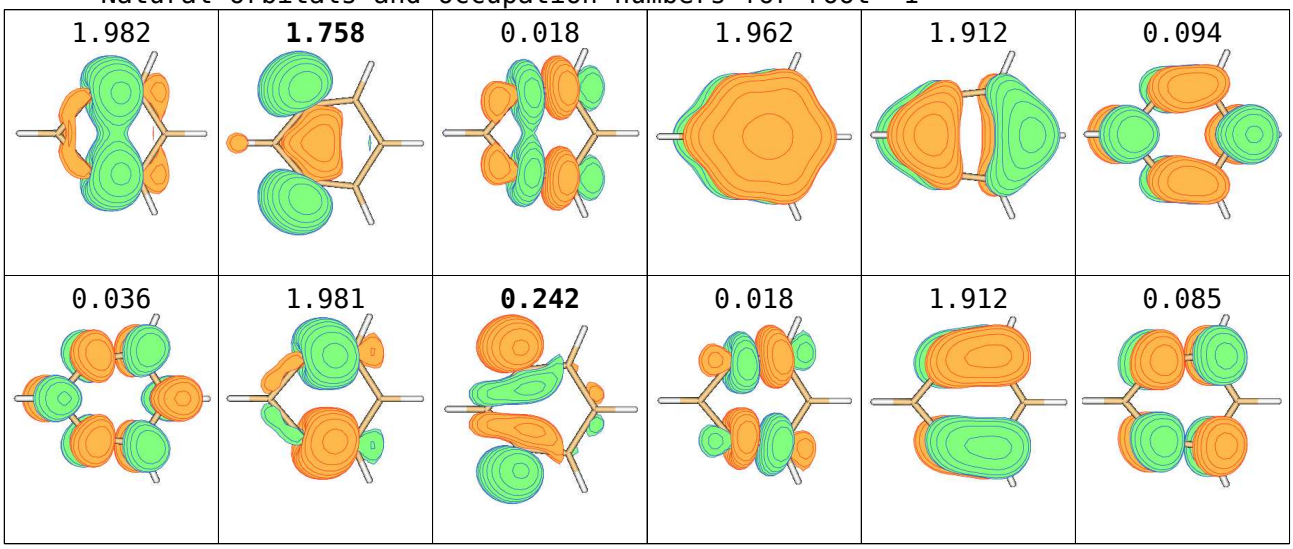
meta-Benzyne (C_{2v})

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	3.03066
3	C4	0.00000	1.17371	0.76191
4	C5	0.00000	1.03264	2.13128
5	H6	0.00000	0.00000	-1.08340
6	H7	0.00000	2.15384	0.31012
7	H8	0.00000	0.00000	4.10583
8	C4	0.00000	-1.17371	0.76191
9	C5	0.00000	-1.03264	2.13128
10	H7	0.00000	-2.15384	0.31012

Natural orbitals and occupation numbers for root 1



Vibrational frequencies (cm-1)

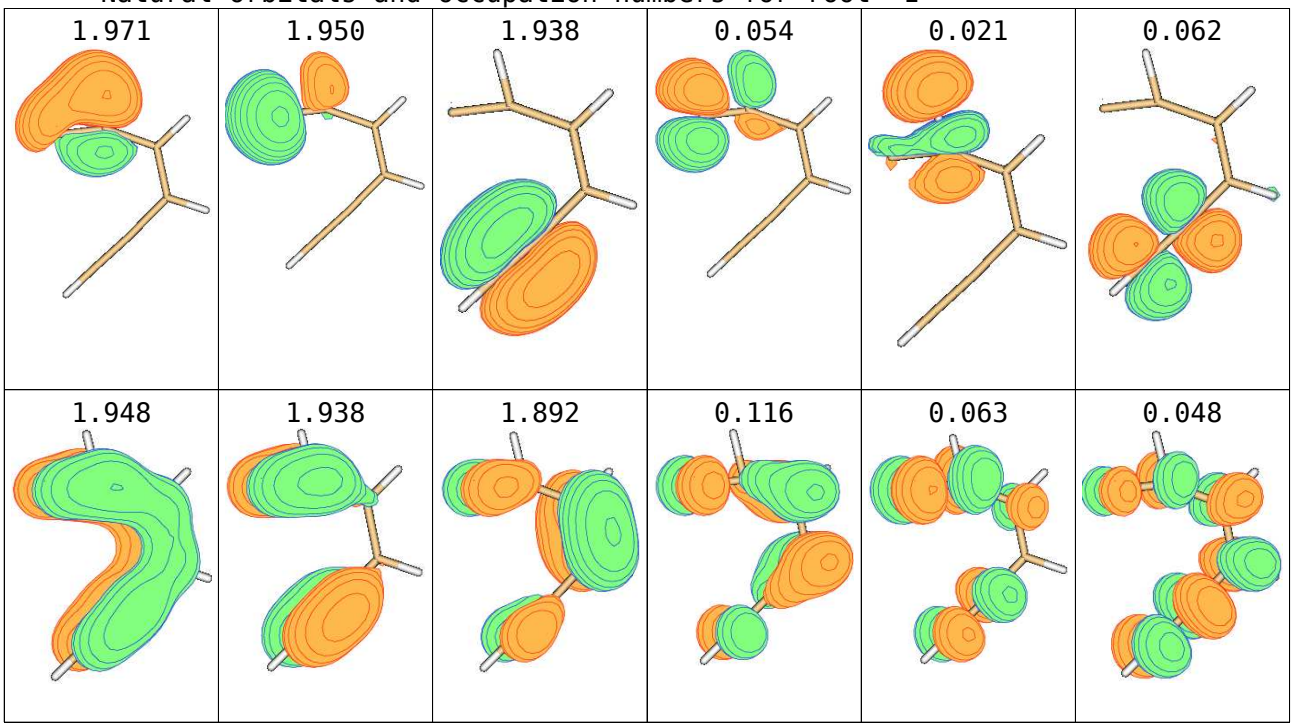
403.75
484.77
502.68
603.89
613.31
802.42
882.69
900.10
921.32
996.90
1007.40
1050.50
1150.39
1173.65
1279.84
1364.86
1474.65
1518.87
1612.14
1675.13
3307.52

```
  3337.58
  3344.86
  3398.95
 -------------------------------
```

TS_7 (C_s)

```
 ----------------------------------------
No.  Label     X         Y         Z
 ----------------------------------------
 1   C1       0.00000   0.00000   0.00000
 2   C2       0.00000   0.00000   1.29282
 3   C3       0.62239   0.00000   2.58936
 4   C4       1.96903   0.00000   2.71922
 5   C5       2.83275   0.00000   1.59437
 6   C6       3.52832   0.00000   0.59976
 7   H7      -0.00568   0.00000   3.46664
 8   H8       2.40857   0.00000   3.70632
 9   H9       4.13985   0.00000  -0.26746
10   H10     -1.12908   0.00000   1.12977
 ----------------------------------------

 Natural orbitals and occupation numbers for root  1
```




```
 -------------------------------
 Vibrational frequencies (cm-1)
  i 225.70
    119.66
    141.85
    248.24
    317.83
    338.55
    544.52
    569.16
    587.12
    608.61
```

```
  738.73
  873.15
  907.24
  966.15
 1051.20
 1316.89
 1526.22
 1709.31
 1994.80
 2238.09
 2467.56
 3327.22
 3354.07
 3605.54
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```

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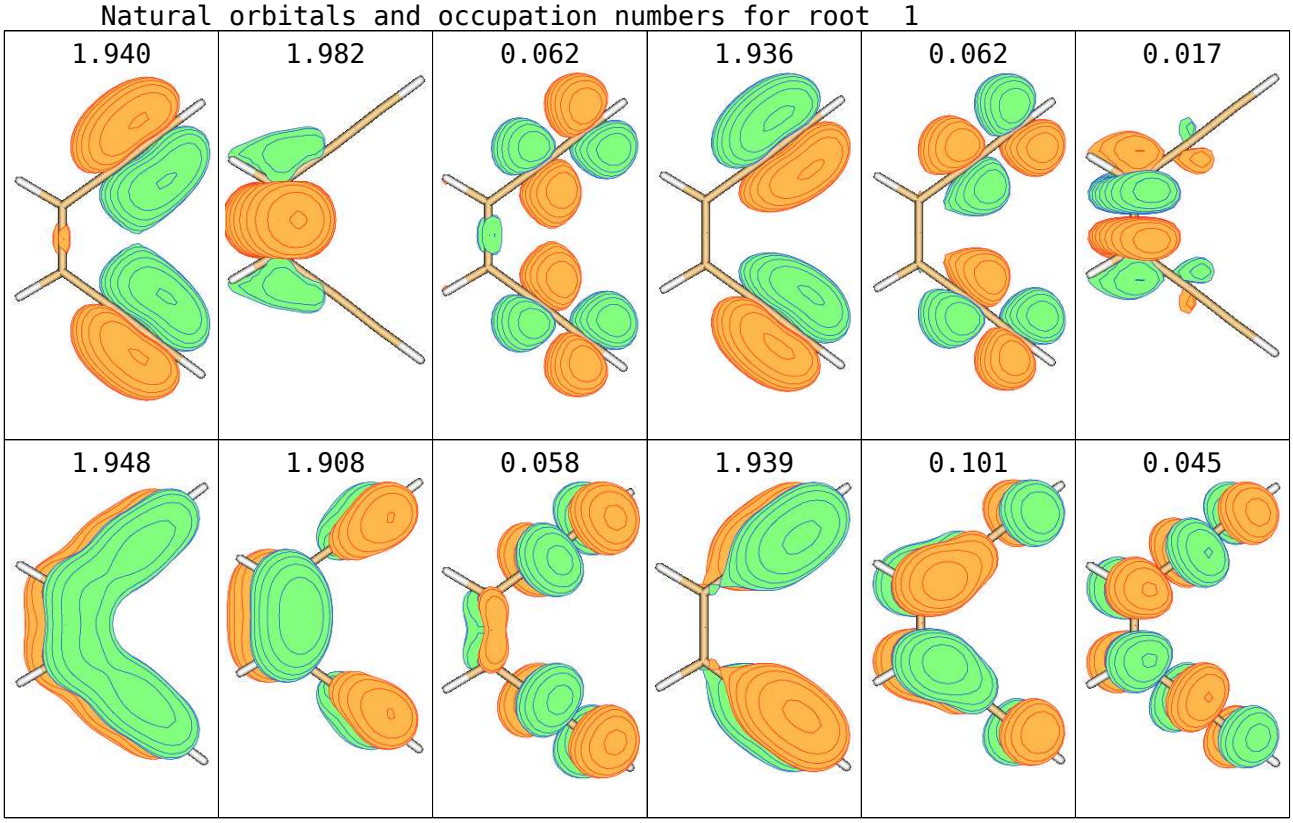
cis-HED (C_{2v})

No.	Label	X	Y	Z
1	C3	0.67720	0.00000	0.00000
2	C4	1.49757	0.00000	1.15540
3	C5	2.24032	0.00000	2.11243
4	H6	1.18903	0.00000	-0.96006
5	H7	2.87380	0.00000	2.96897
6	C3	-0.67720	0.00000	0.00000
7	C4	-1.49757	0.00000	1.15540
8	C5	-2.24032	0.00000	2.11243
9	H6	-1.18903	0.00000	-0.96006
10	H7	-2.87380	0.00000	2.96897

Natural orbitals and occupation numbers for root 1

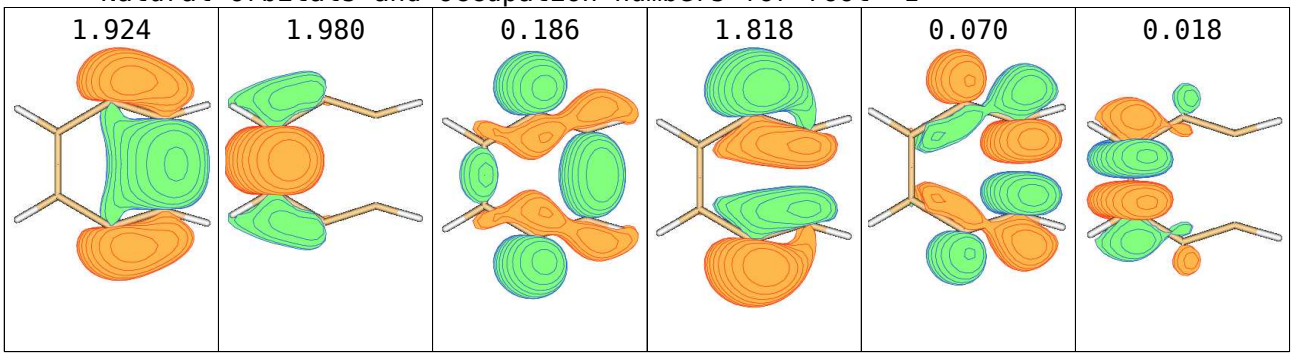


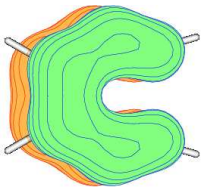
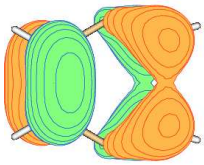
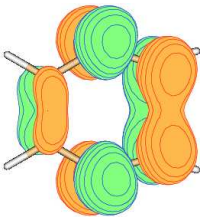
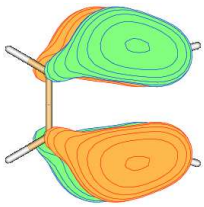
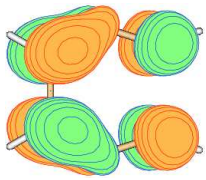
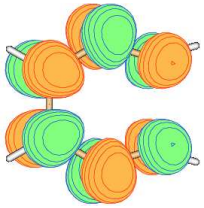
```
------------------------------
Vibrational frequencies (cm-1)
   102.01
   209.48
   220.81
   316.55
   401.46
   544.41
   560.49
   566.78
   578.60
   576.54
   730.99
   784.23
   892.27
  1003.45
  1058.97
  1305.01
  1510.19
  1643.10
  2232.67
  2240.32
  3316.21
  3334.97
  3606.48
  3607.33
------------------------------
```

TS_8 (C_{2v})

No.	Label	X	Y	Z
1	C3	0.69686	0.00000	-0.00104
2	C4	1.37044	0.00000	1.22724
3	C5	1.00975	0.00000	2.43997
4	H6	1.21411	0.00000	-0.94728
5	H7	1.29120	0.00000	3.47101
6	C3	-0.69686	0.00000	-0.00104
7	C4	-1.37044	0.00000	1.22724
8	C5	-1.00975	0.00000	2.43997
9	H6	-1.21411	0.00000	-0.94728
10	H7	-1.29120	0.00000	3.47101

Natural orbitals and occupation numbers for root 1



1.949	1.899	0.075	1.922	0.111	0.046
					

```
--------------------------------
Vibrational frequencies (cm-1)
 i 776.57
   352.39
   427.03
   487.83
   545.54
   601.02
   644.61
   681.72
   742.01
   818.97
   875.68
   975.03
  1025.45
  1042.28
  1151.17
  1212.13
  1485.18
  1430.84
  1692.80
  1864.90
  3345.10
  3362.79
  3465.57
  3472.25
--------------------------------
```

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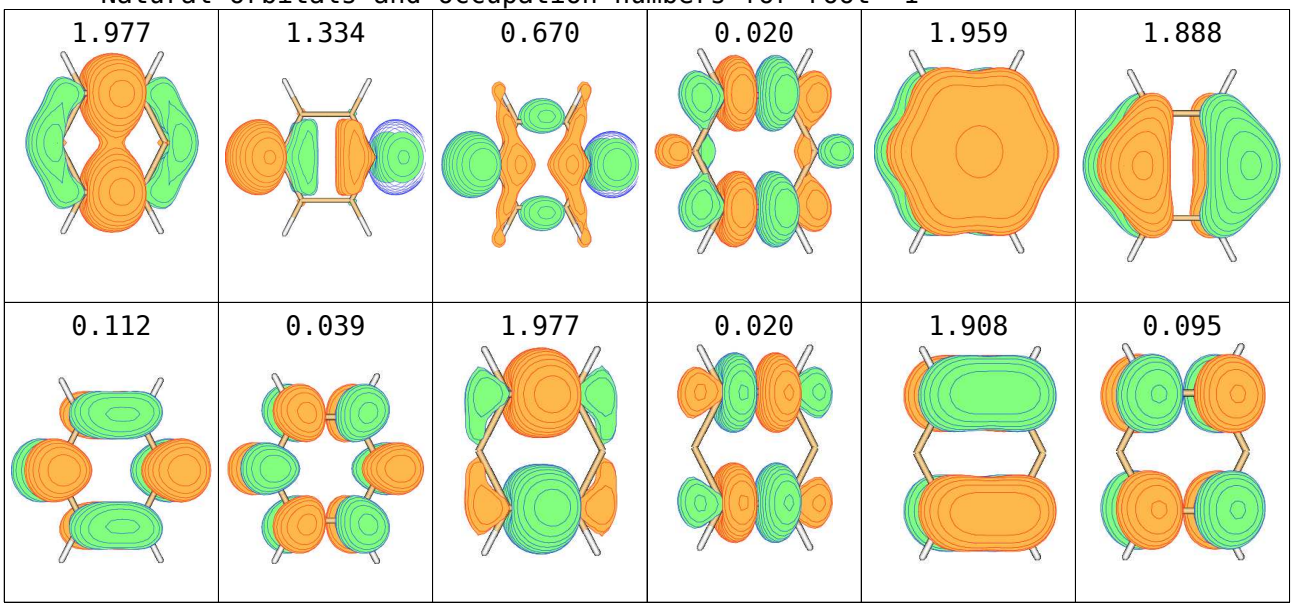
para-Benzyne (C_{2v})

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	2.70759
3	C4	0.00000	1.20743	0.63606
4	C5	0.00000	1.20743	2.07154
5	H6	0.00000	2.15933	0.12760
6	H7	0.00000	2.15932	2.58005
7	C4	0.00000	-1.20743	0.63606
8	C5	0.00000	-1.20743	2.07154
9	H6	0.00000	-2.15933	0.12760
10	H7	0.00000	-2.15932	2.58005

Natural orbitals and occupation numbers for root 1



Vibrational frequencies (cm-1)

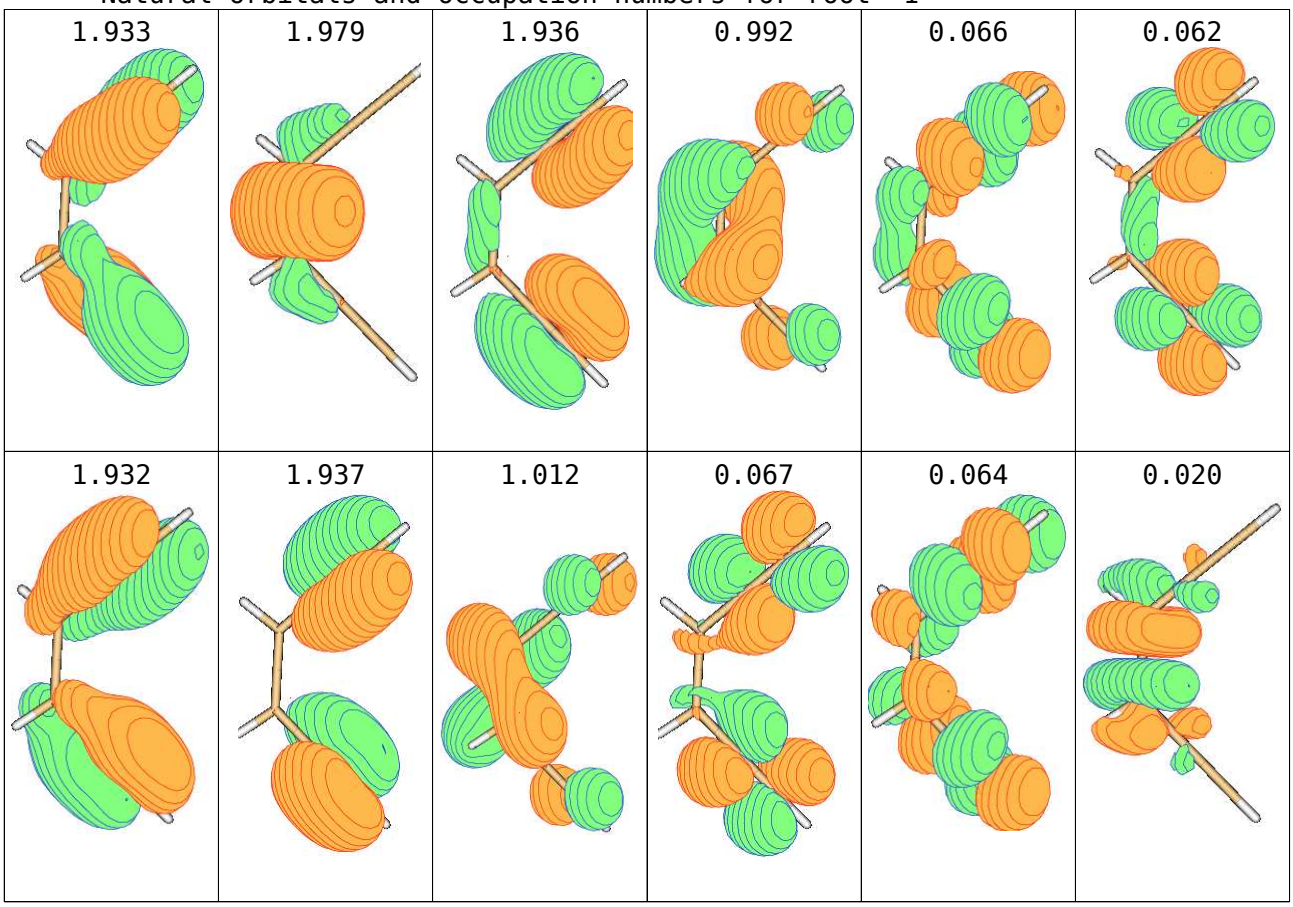
438.49
474.32
606.59
652.58
654.56
749.06
787.06
936.16
970.18
980.25
1007.45
1007.62
1096.63
1188.07
1235.30
1359.86
1397.13
1407.57
1540.58
1707.01
3338.33
3338.91
3353.44
3354.64

TS_9 (C_s)

No.	Label	X	Y	Z
1	C3	0.73855	0.00000	0.00171
2	C4	1.47239	-0.81680	0.83731
3	C5	2.11233	-1.54436	1.58985
4	H6	1.26515	0.68068	-0.65569

5	H7	2.66496	-2.17543	2.23827
6	C3	-0.73855	0.00000	-0.00171
7	C4	-1.47239	-0.81680	-0.83731
8	C5	-2.11233	-1.54436	-1.58985
9	H6	-1.26515	0.68068	0.65569
10	H7	-2.66496	-2.17543	-2.23827

Natural orbitals and occupation numbers for root 1



Vibrational frequencies (cm-1)

i 1038.49
98.39
198.09
220.99
337.72
385.79
423.04
427.03
443.42
525.87
546.16
546.28
633.51
912.00
1062.93
1170.76
1383.64
1421.67
2082.06

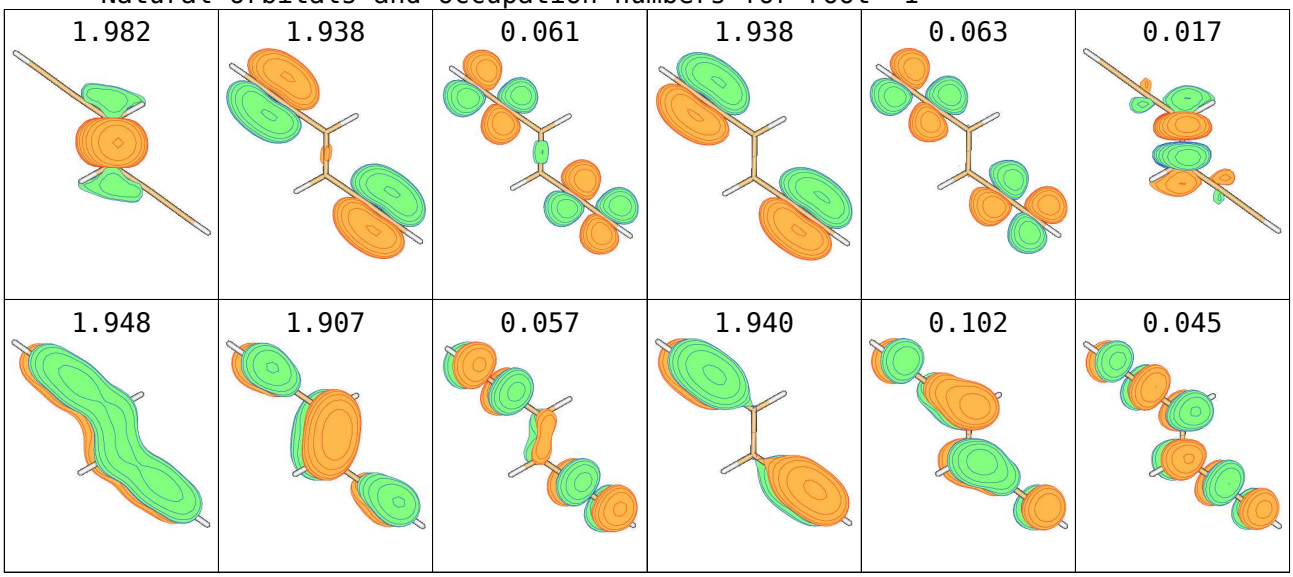
2090.83
3319.87
3321.29
3603.49
3603.66

---

trans-HED (C_{2h})

No.	Label	X	Y	Z
1	C3	0.67624	0.00000	-0.01109
2	C4	1.46593	0.00000	1.16934
3	C5	2.17155	0.00000	2.15635
4	H6	1.19544	0.00000	-0.95895
5	H7	2.77903	0.00000	3.02529
6	C3	-0.67624	0.00000	0.01109
7	C4	-1.46593	0.00000	-1.16934
8	C5	-2.17155	0.00000	-2.15635
9	H6	-1.19544	0.00000	0.95895
10	H7	-2.77903	0.00000	-3.02529

Natural orbitals and occupation numbers for root 1



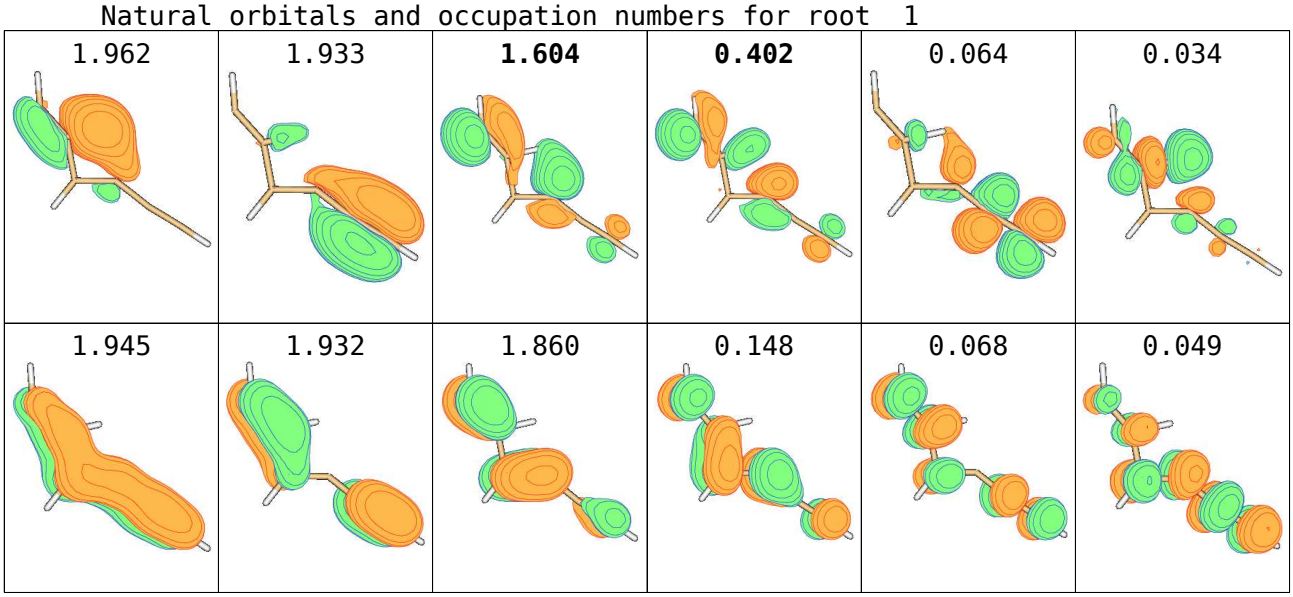
Vibrational frequencies (cm-1)
116.54
121.13
218.79
314.30
469.40
474.93
511.27
552.83
555.10
582.45
583.59
848.18
1021.03

1048.65
1048.96
1372.34
1374.92
1671.46
2229.14
2240.68
3322.15
3329.30
3604.57
3604.82

TS_{10} (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.35356
3	C3	0.82084	0.00000	2.45271
4	C4	1.43338	0.00000	3.51185
5	C5	-1.39984	0.00000	-0.28570
6	C6	-2.33846	0.00000	-1.16961
7	H7	-1.67804	0.00000	0.93059
8	H8	1.99736	0.00000	4.41079
9	H9	-3.40554	0.00000	-1.26957
10	H10	0.83784	0.00000	-0.68669

Natural orbitals and occupation numbers for root 1



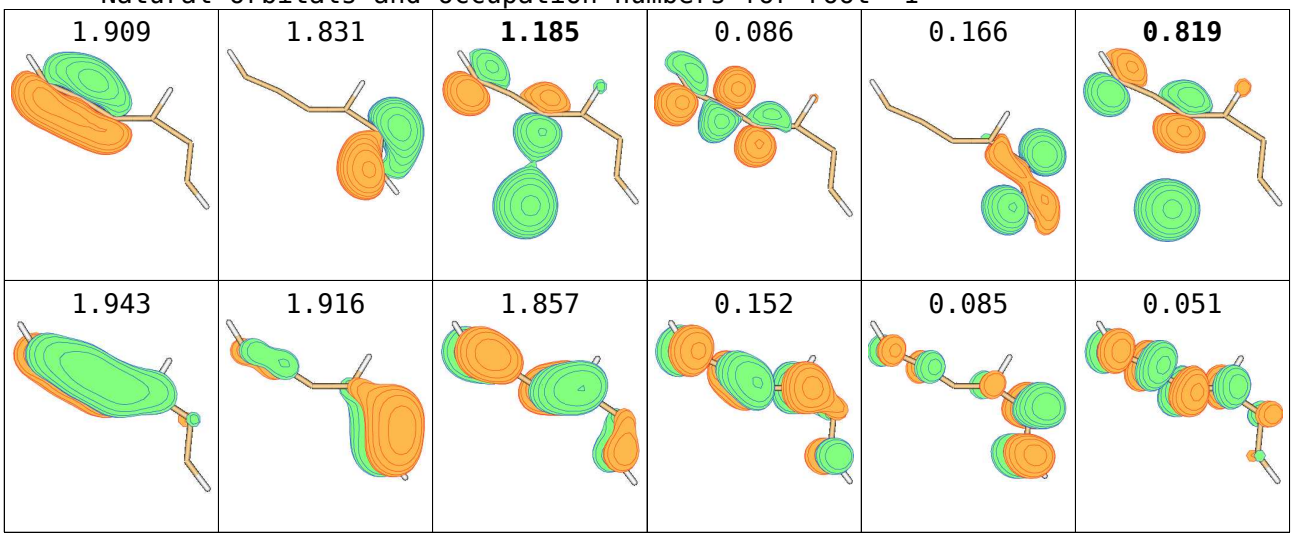
Vibrational frequencies (cm-1)
i 1781.01
131.88
138.10
291.21
345.73
466.15
513.92

```
  533.10
  541.63
  555.81
  624.36
  837.11
  862.14
  930.23
  989.58
 1083.90
 1335.52
 1660.30
 1730.21
 1885.60
 2150.83
 3323.06
 3459.38
 3603.05
-------------------------------
```

TS_{11} (C_s)

```
-----------------------------------------
No.  Label     X          Y          Z
-----------------------------------------
 1   C1       0.00000    0.00000    0.00000
 2   C2       0.00000    0.00000    1.32890
 3   C3       1.18966    0.00000    2.11044
 4   C4       2.17794    0.00000    2.81187
 5   C5      -0.57009    0.00000   -1.20577
 6   C6      -0.97036    0.00000   -2.37354
 7   H7      -0.94533    0.00000    1.86433
 8   H8       3.05352    0.00000    3.40972
 9   H9      -1.36876    0.00000   -3.35634
10   H10      3.51009    0.00000   -3.27399
-----------------------------------------
```

Natural orbitals and occupation numbers for root 1



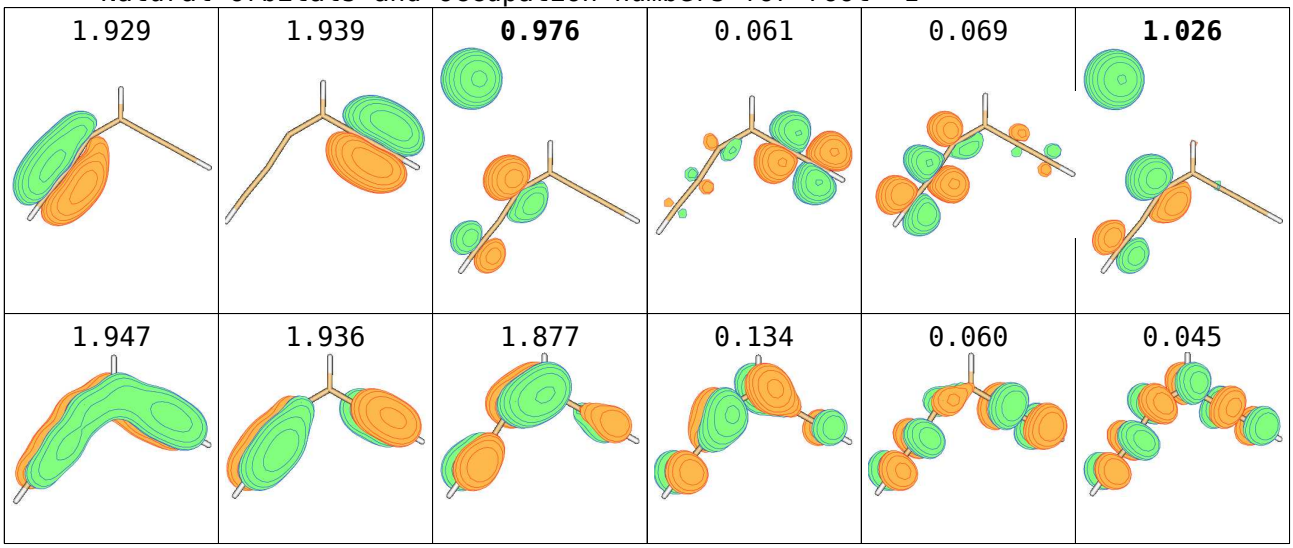

```
-------------------------------
Vibrational frequencies (cm-1)
  i 29.02
    14.24
```

```
    18.33
   109.47
   130.21
   233.96
   311.42
   429.89
   449.84
   493.96
   510.23
   528.02
   549.55
   580.32
   769.10
   926.62
  1073.55
  1386.59
  1737.20
  2066.99
  2236.55
  3287.10
  3601.23
  3606.92
 -------------------------------
```

TS_{12} (C_s)

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.33105
3	C3	1.19886	0.00000	2.10115
4	C4	2.21038	0.00000	2.76947
5	C5	0.61441	0.00000	-1.18768
6	C6	1.05095	0.00000	-2.34107
7	H7	-0.94206	0.00000	1.86459
8	H8	3.10123	0.00000	3.34445
9	H9	1.48765	0.00000	-3.30749
10	H10	-4.37363	0.00000	0.39087

Natural orbitals and occupation numbers for root 1



```
------------------------------
Vibrational frequencies (cm-1)
  i 17.86
    10.63
    91.81
   234.17
   392.17
   493.85
   578.88
   667.12
   861.24
  1041.70
  1412.05
  1733.93
  2066.43
  2229.95
  3317.95
  3601.93
  3606.86
    23.46
   216.10
   321.84
   487.22
   534.92
   549.77
   792.14
------------------------------
```

IV (C_s)

```
-----------------------------------------
No.  Label     X          Y          Z
-----------------------------------------
 1   C1       0.00000    0.00000    0.00000
 2   C2       0.00000    0.00000    1.33069
 3   C3       1.19796    0.00000    2.10155
 4   C4       2.20721    0.00000    2.77370
 5   C5       0.58671    0.00000   -1.19986
 6   C6       0.99833    0.00000   -2.36286
 7   H7      -0.94031    0.00000    1.86722
 8   H8       3.09649    0.00000    3.35051
 9   H9       1.41155    0.00000   -3.33967
-----------------------------------------
```

Natural orbitals and occupation numbers for root 1

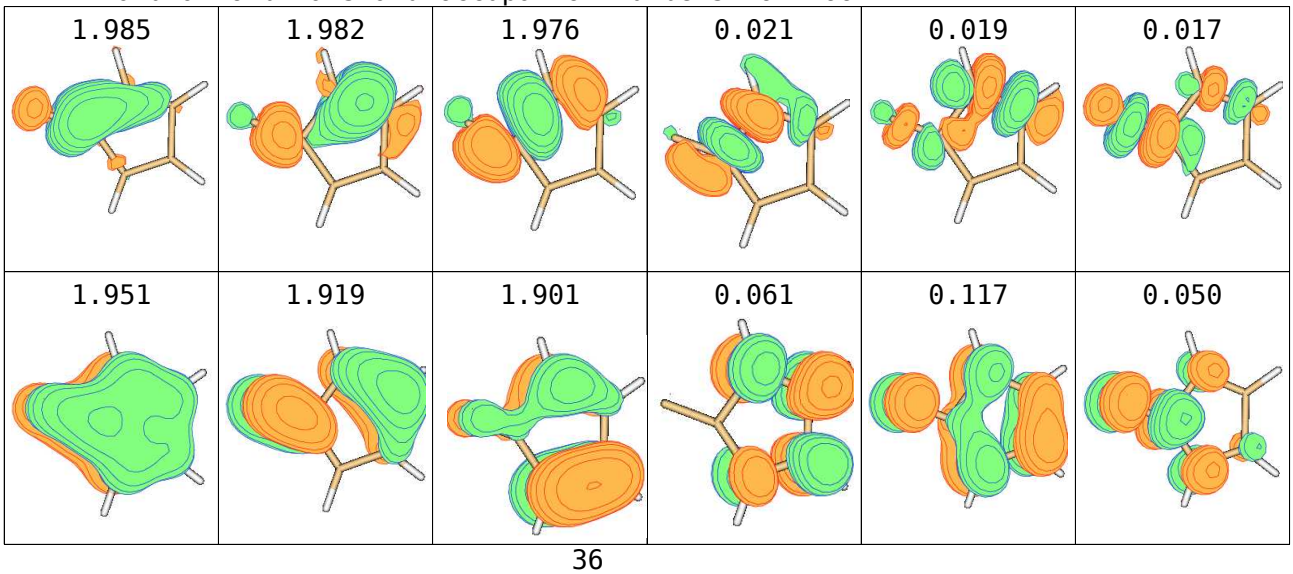
1.929	1.939	1.002	0.068	0.061	/
1.947	1.936	1.877	0.134	0.060	0.045

```
------------------------------
Vibrational frequencies (cm-1)
    89.14
   212.67
   232.99
   320.56
   391.18
   488.52
   492.43
   534.79
   549.44
   578.62
   792.05
   665.90
   861.82
  1042.23
  1412.54
  1733.90
  2067.09
  2229.65
  3318.36
  3601.74
  3606.76
------------------------------
```

TS_{13} (o-Bz => cyclopentadienylidene) (C_s)

```
----------------------------------------
No.  Label     X          Y          Z
----------------------------------------
 1   C1       0.00000    0.00000    0.00000
 2   C2       0.00000    0.00000    2.27419
 3   C3       0.89369    0.00000    3.29834
 4   C4       2.25252    0.00000    2.77475
 5   C5       2.22193    0.00000    1.41477
 6   C6       0.82814    0.00000    1.01475
 7   H7      -1.07313    0.00000    2.31757
 8   H8       0.63113    0.00000    4.34353
 9   H9       3.14651    0.00000    3.37729
10   H10      3.04864    0.00000    0.72766
----------------------------------------
```

Natural orbitals and occupation numbers for root 1



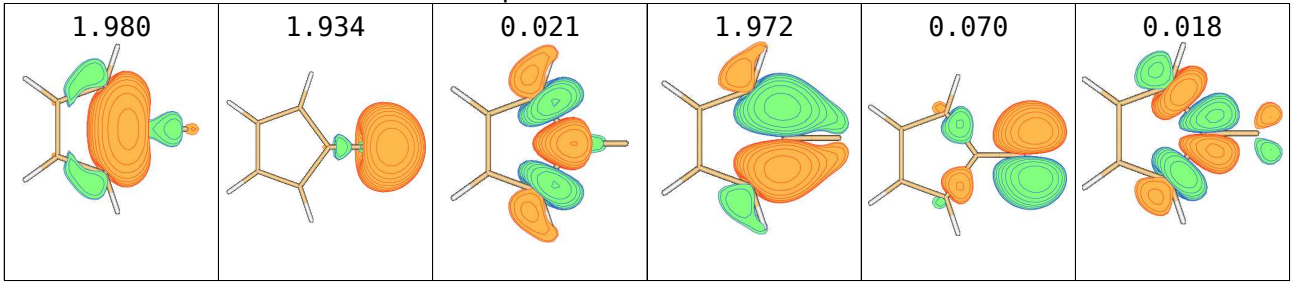
```
------------------------------
Vibrational frequencies (cm-1)
 i 378.62
   191.65
   513.86
   588.74
   635.13
   667.85
   722.54
   762.85
   865.75
   936.82
   962.07
  1011.90
  1084.14
  1194.05
  1200.34
  1349.11
  1473.39
  1527.64
  1641.49
  1933.84
  3345.98
  3363.83
  3394.53
  3427.79
------------------------------
```

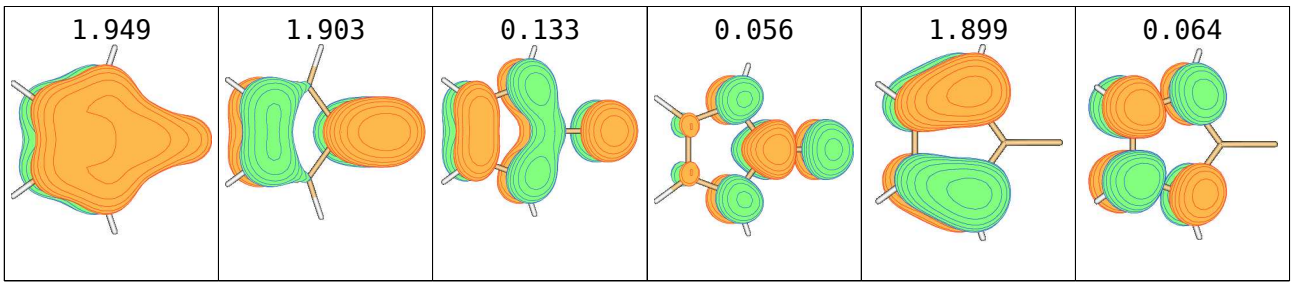
Cyclopentadienylidene (CPDene) (C_{2v})

Cartesian coordinates in Angstrom:

No.	Label	X	Y	Z
1	C1	0.00000	0.00000	0.00000
2	C2	0.00000	0.00000	1.31614
3	C3	1.18676	0.00000	-0.87932
4	C4	0.72946	0.00000	-2.15792
5	H5	2.20364	0.00000	-0.53162
6	H6	1.34912	0.00000	-3.04016
7	C3	-1.18676	0.00000	-0.87932
8	C4	-0.72946	0.00000	-2.15792
9	H5	-2.20364	0.00000	-0.53162
10	H6	-1.34912	0.00000	-3.04016

Natural orbitals and occupation numbers for root 1






```
sym 1:   1.979935   1.933841   0.021414
sym 2:   1.971648   0.070185   0.017767
sym 3:   1.949272   1.903206   0.132982   0.055984
sym 4:   1.899530   0.064237

-------------------------------
Vibrational frequencies (cm-1)
   199.25
   206.39
   535.49
   586.85
   670.48
   718.68
   757.02
   854.23
   887.65
   926.69
   931.86
  1049.44
  1058.66
  1184.48
  1186.20
  1400.41
  1483.55
  1592.69
  1674.49
  1739.51
  3351.47
  3364.11
  3392.57
  3396.14
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```