

Supplementary data for article:

Baranac-Stojanović, M.; Stojanović, M. H-1 NMR Chemical Shifts of Cyclopropane and Cyclobutane: A Theoretical Study. *Journal of Organic Chemistry* **2013**, 78 (4), 1504–1507.  
<https://doi.org/10.1021/jo3025863>

## Supporting Information for

# <sup>1</sup>H NMR Chemical Shifts of Cyclopropane and Cyclobutane: a Theoretical Study

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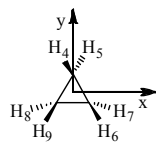
**Table S1.**  $\text{CH}_{\text{main}}^a$  contributions (ppm) to  $\sigma(\text{H})$  obtained by the NCS analysis of proton shielding tensor.

Compound		$\text{CH}_{\text{main}}$ (iso) <sup>b</sup>	$\sigma^c$	$\delta^d$	exp
$\text{C}_2\text{H}_6$ ( $D_{3d}$ )		25.91	31.01	0.96	0.86
$\text{C}_3\text{H}_8$ ( $C_{2v}$ )	$\text{CH}_2$	26.44	30.54	1.43	1.33
<i>i</i> - $\text{C}_4\text{H}_{10}$ ( $C_{3v}$ )	$\text{CH}$	26.69	30.23	1.74	1.56
$\text{C}_3\text{H}_6$ ( $D_{3h}$ )		25.62	31.79	0.18	0.22
$\text{C}_4\text{H}_8$ ( $D_{2d}$ )	$\text{av}^e$	26.28	29.96	2.01	1.98
$\text{C}_6\text{H}_{12}$ ( $D_{3d}$ )	$\text{av}^e$	26.54	30.47	1.50	1.43

<sup>a</sup> Contribution from the C–H bond in which proton is involved. <sup>b</sup> Corresponds to the average of all space orientations. <sup>c</sup> Calculated proton shielding constant.

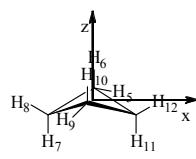
<sup>d</sup> Calculated chemical shift relative to TMS,  $\sigma(\text{TMS}) - \sigma(\text{H})$ ; computed  $\sigma(\text{TMS}) = 31.97$ . <sup>e</sup> Average of axial and equatorial positions.

**Table S2.** Orbital contributions (ppm) to  $\sigma(\text{H-4})$  and  $\sigma(\text{H-6})$  in cyclopropane ( $D_{3h}$ ) obtained by the NCS analysis of proton shielding tensor.<sup>a</sup>

	H-4				H-6			
	$\sigma_{xx}$	$\sigma_{yy}$	$\sigma_{zz}$	$\sigma_{iso}$	$\sigma_{xx}$	$\sigma_{yy}$	$\sigma_{zz}$	$\sigma_{iso}$
C1-C2	0.10	2.56	2.62	1.76	2.04	0.62	2.62	1.76
C1-C3	0.10	2.56	2.62	1.76	0.56	0.16	0.60	0.44
C1-H4	24.68	25.08	27.10	25.62	-0.23	0.31	0.14	0.08
C1-H5	2.63	0.34	2.46	1.81	-0.26	0.36	0.08	0.06
C2-C3	-0.04	0.76	0.60	0.44	1.85	0.81	2.62	1.76
C2-H6	-0.40	0.49	0.14	0.08	24.98	24.78	27.10	25.62
C2-H7	-0.16	0.27	0.08	0.06	0.91	2.05	2.46	1.81
C3-H8	-0.16	0.27	0.08	0.06	0.58	-0.47	0.08	0.06
C3-H9	-0.40	0.49	0.14	0.08	0.76	-0.67	0.14	0.08
core C1	0.10	0.06	0.40	0.19	-0.06	0.02	-0.05	-0.03
core C2	-0.05	0.01	-0.05	-0.03	0.07	0.09	0.40	0.19
core C3	-0.05	0.01	-0.05	-0.03	0.05	-0.09	-0.05	-0.03
total	26.33	32.89	36.15	31.79	31.25	27.97	36.15	31.79
CC <sub>all</sub>	0.16	5.88	5.84	3.96	4.45	1.59	5.84	3.96
CH <sub>same side</sub>	-0.80	0.98	0.28	0.16	0.53	-0.36	0.28	0.16
CH <sub>other side</sub>	2.31	0.88	2.62	1.93	1.23	1.94	2.62	1.93
CH <sub>other all</sub>	1.51	1.86	2.90	2.09	1.76	1.58	2.90	2.09

<sup>a</sup>  $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{zz}$  and  $\sigma_{iso}$  denote shielding contributions when a magnetic field is applied along the x, y and z axis, respectively, and the average of all space orientations,  $\sigma_{iso} = 1/3(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$ .

**Table S3.** Orbital contributions (ppm) to  $\sigma(\text{H-11}_{\text{ax}})$  and  $\sigma(\text{H-12}_{\text{eq}})$  in cyclobutane ( $D_{2d}$ ) obtained by the NCS analysis of proton shielding tensor.<sup>a</sup>



	$\text{H}_{\text{ax}}$				$\text{H}_{\text{eq}}$			
	$\sigma_{\text{xx}}$	$\sigma_{\text{yy}}$	$\sigma_{\text{zz}}$	$\sigma_{\text{iso}}$	$\sigma_{\text{xx}}$	$\sigma_{\text{yy}}$	$\sigma_{\text{zz}}$	$\sigma_{\text{iso}}$
C1-C2	0.46	-0.31	-0.53	-0.13	0.42	-0.34	-0.93	-0.28
C1-C4	1.96	0.88	1.05	1.29	1.93	0.11	0.81	0.95
C1-H5	-0.03	0.04	-0.16	-0.05	0.40	0.02	0.11	0.18
C1-H6	-0.07	-0.09	0.00	-0.05	0.48	-0.16	-0.40	-0.02
C2-C3	0.46	-0.31	-0.53	-0.13	0.42	-0.34	-0.93	-0.28
C2-H7	0.55	-0.25	-0.16	0.05	0.35	-0.11	-0.13	0.04
C2-H8	0.24	-0.11	-0.45	-0.10	0.25	-0.08	-0.36	-0.06
C3-C4	1.96	0.88	1.05	1.29	1.93	0.11	0.81	0.95
C3-H9	-0.03	0.04	-0.16	-0.05	0.40	0.02	0.11	0.18
C3-H10	-0.07	-0.09	0.00	-0.05	0.48	-0.16	-0.40	-0.02
C4-H11	25.02	24.81	28.69	26.17	0.71	3.18	1.77	1.89
C4-H12	0.12	2.71	1.65	1.49	27.28	24.66	27.26	26.40
core C1	-0.02	-0.01	-0.05	-0.03	0.00	0.00	-0.07	-0.02
core C2	0.03	-0.06	-0.08	-0.04	0.02	-0.05	-0.07	-0.03
core C3	-0.02	-0.01	-0.05	-0.03	0.00	0.00	-0.07	-0.02
core C4	-0.02	-0.03	0.56	0.17	0.24	0.14	0.46	0.28
total	30.55	28.09	30.83	29.82	35.33	27.01	27.98	30.11
CC <sub>all</sub>	4.84	1.14	1.04	2.34	4.70	-0.44	-0.23	1.34
CH <sub>same side</sub>	0.49	-0.16	-0.48	-0.05	1.22	-0.39	-1.16	-0.11
CH <sub>other side</sub>	0.23	2.43	1.21	1.29	1.87	3.11	1.85	2.28
CH <sub>other all</sub>	0.72	2.27	0.73	1.24	3.09	2.72	0.69	2.17

<sup>a</sup>  $\sigma_{\text{xx}}$ ,  $\sigma_{\text{yy}}$ ,  $\sigma_{\text{zz}}$  and  $\sigma_{\text{iso}}$  denote shielding contributions when a magnetic field is applied along the x, y and z axis, respectively, and the average of all space orientations,  
 $\sigma_{\text{iso}} = 1/3(\sigma_{\text{xx}} + \sigma_{\text{yy}} + \sigma_{\text{zz}})$ .

**Table S4.** Orbital contributions (ppm) to the average  $\sigma(\text{H})$  in cyclobutane ( $D_{2d}$ ) obtained by the NCS analysis of proton shielding tensor.<sup>a</sup>

Contribution	$\sigma_{xx}$	$\sigma_{yy}$	$\sigma_{zz}$	$\sigma_{iso}$
CC <sub>all</sub>	4.77	0.35	0.40	1.84
CH <sub>main</sub>	26.15	24.74	27.98	26.28
CH <sub>same side</sub>	0.85	-0.28	-0.82 <sup>b</sup>	-0.08
CH <sub>other side</sub>	1.05	2.77	1.53	1.78
CH <sub>other all</sub>	1.91	2.49	0.71	1.70

<sup>a</sup>  $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{zz}$  and  $\sigma_{iso}$  denote shielding contributions when a magnetic field is applied along the x, y and z axis, respectively, and the average of all space orientations,  $\sigma_{iso} = 1/3(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$ . <sup>b</sup> The corresponding contribution for  $D_{4h}$  form is -1.10 ppm.

**Table S5.** Orbital contributions (ppm) to  $\sigma(\text{H})$  in cyclopropane and cyclobutane obtained by the NCS analysis of proton shielding tensor.<sup>a</sup>

Contribution	C <sub>3</sub> H <sub>6</sub> ( $D_{3h}$ )			C <sub>4</sub> H <sub>8</sub> ( $D_{2d}$ ) av <sup>b</sup>		
	$(\sigma_{xx} + \sigma_{yy})/2$	$\sigma_{zz}$	$\sigma_{iso}$	$(\sigma_{xx} + \sigma_{yy})/2$	$\sigma_{zz}$	$\sigma_{iso}$
CH <sub>main</sub>	24.88	27.10	25.62	25.44	27.98	26.28
CH <sub>same side</sub>	0.09	0.28	0.16	0.28	-0.82	-0.08
CH <sub>other side</sub>	1.60	2.62	1.93	1.91	1.53	1.78
CH <sub>other all</sub>	1.69	2.90	2.09	2.19	0.71	1.70
CC <sub>all</sub>	3.02	5.84	3.96	2.56	0.40	1.84

<sup>a</sup>  $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{zz}$  and  $\sigma_{iso}$  denote shielding contributions when a magnetic field is applied along the x, y and z axis, respectively, and the average of all space orientations,

$\sigma_{iso} = 1/3(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$ . <sup>b</sup> Average values for  $D_{2d}$  form.

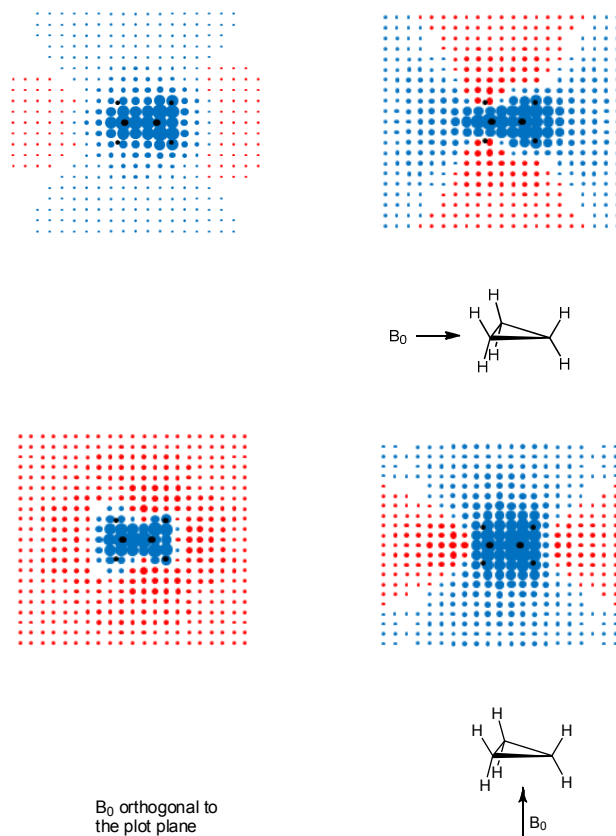
## Comparison of orbital contributions to cyclopropane, cyclobutane and cyclohexane proton chemical shifts

**Table S6.** Orbital contributions (ppm) to  $\sigma(\text{H})$  in cyclopropane and to the average<sup>a</sup>  $\sigma(\text{H})$  in cyclobutane and cyclohexane obtained by the NCS analysis of proton shielding tensor.<sup>b</sup>

Contribution	$\text{C}_3\text{H}_6$ ( $D_{3h}$ ) ( $\delta$ 0.22)			$\text{C}_4\text{H}_8$ ( $D_{2d}$ ) average ( $\delta$ 1.98)			$\text{C}_6\text{H}_{12}$ ( $D_{3d}$ ) average ( $\delta$ 1.43)		
	$\sigma_{xx} + \sigma_{yy}$	$\sigma_{zz}$	$\sigma_{\text{iso}}$	$\sigma_{xx} + \sigma_{yy}$	$\sigma_{zz}$	$\sigma_{\text{iso}}$	$\sigma_{xx} + \sigma_{yy}$	$\sigma_{zz}$	$\sigma_{\text{iso}}$
CC <sub>all</sub>	6.04	5.84	3.96	5.12	0.40	1.84	3.98	1.88	1.95
CH <sub>main</sub>	49.76	27.10	25.62	50.89	27.98	26.28	52.08	27.53	26.54
CH <sub>same side</sub>	0.18	0.28	0.16	0.57	-0.82	-0.08	1.15	-0.86	0.09
CH <sub>other side</sub>	3.19	2.62	1.93	3.82	1.53	1.78	4.26	0.91	1.72
CH <sub>other all</sub>	3.37	2.90	2.09	4.40	0.71	1.70	5.41	0.05	1.81
total <sup>c</sup>	59.17	35.84	31.67	60.41	29.09	29.82	61.47	29.46	30.30

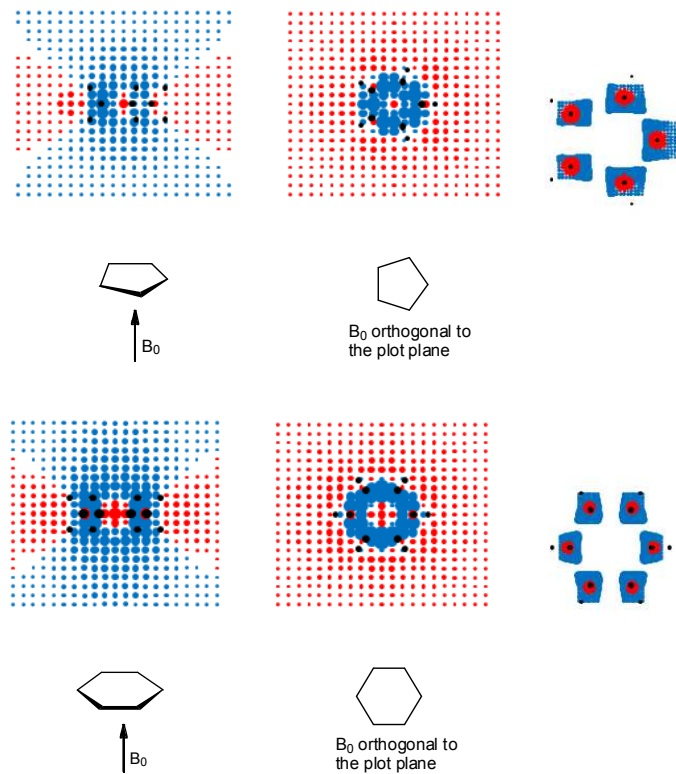
<sup>a</sup> Based on equal proportion of the two conformations. <sup>b</sup>  $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{zz}$  and  $\sigma_{\text{iso}}$  denote shielding contributions when a magnetic field is applied along the x, y and z axis, respectively, and the average of all space orientations,  $\sigma_{\text{iso}} = 1/3(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$ . <sup>c</sup> Core electron contributions are not included in these values.

An assessment of the CC framework effects coming from the perpendicular orientation of a ring with respect to a magnetic field,  $5.84/3 \approx 1.9$  for cyclopropane,  $0.4/3 \approx 0.1$  for cyclobutane and  $1.88/3 \approx 0.6$  for the cyclohexane chair conformation, is in perfect agreement with experimentally observed chemical shift differences (Table S6). Thus, cyclobutane hydrogen is by  $\sim 1.8$  ppm less shielded than cyclopropane proton and by  $\sim 0.5$  ppm less shielded than cyclohexane hydrogen by the CC framework. Likewise, cyclohexane proton is by  $\sim 1.3$  ppm less shielded than proton in cyclopropane. Can analysis of chemical shift differences between cycloalkanes be simplified and the observed differences accounted for by the CC framework effects exerted in the mentioned orientation? The answer is: No. It is the fact that cyclopropane C–H bonds shield a considered H by as much as 2.9 ppm in the perpendicular orientation providing a shielding contribution of  $\sim 1$  ppm to the average chemical shift, seen in an NMR experiment. The corresponding contributions for cyclobutane and cyclohexane hydrogens are 0.24 and negligible 0.02 ppm, respectively. While a large difference in orbital contributions to cyclopropane and cyclobutane proton chemical shifts arises from perpendicular orientation of molecules relative to a magnetic field,  $\sigma_{zz}(\text{C}_3\text{H}_6) - \sigma_{zz}(\text{C}_4\text{H}_8)$ , that is  $35.84 - 29.09 = 6.75/3 \approx 2.3$  ppm compared to  $(\sigma_{xx} + \sigma_{yy})(\text{C}_4\text{H}_8) - (\sigma_{xx} + \sigma_{yy})(\text{C}_3\text{H}_6)$ , that is  $60.41 - 59.17 = 1.24/3 \approx 0.4$  ppm observed for parallel orientations where  $\text{C}_4\text{H}_8$  is more shielded, this is not the case with cyclobutane and cyclohexane. Here, larger differences come from parallel orientations,  $(\sigma_{xx} + \sigma_{yy})(\text{C}_6\text{H}_{12}) - (\sigma_{xx} + \sigma_{yy})(\text{C}_4\text{H}_8)$ , that is  $61.47 - 60.41 = 1.06/3 \approx 0.4$  ppm compared to  $\sigma_{zz}(\text{C}_6\text{H}_{12}) - \sigma_{zz}(\text{C}_4\text{H}_8)$ , that is  $29.46 - 29.09 = 0.37/3 \approx 0.1$  ppm arising from perpendicular positions. The only deshielding candidate in cyclobutane, C–H bonds located at the same side as the considered proton, deshielding of which arises from perpendicular orientation, exists in cyclohexane too, with almost equal deshielding magnitude (Table S6). For these reasons, it was not possible to isolate any specific effect responsible for high chemical shift of cyclobutane protons.

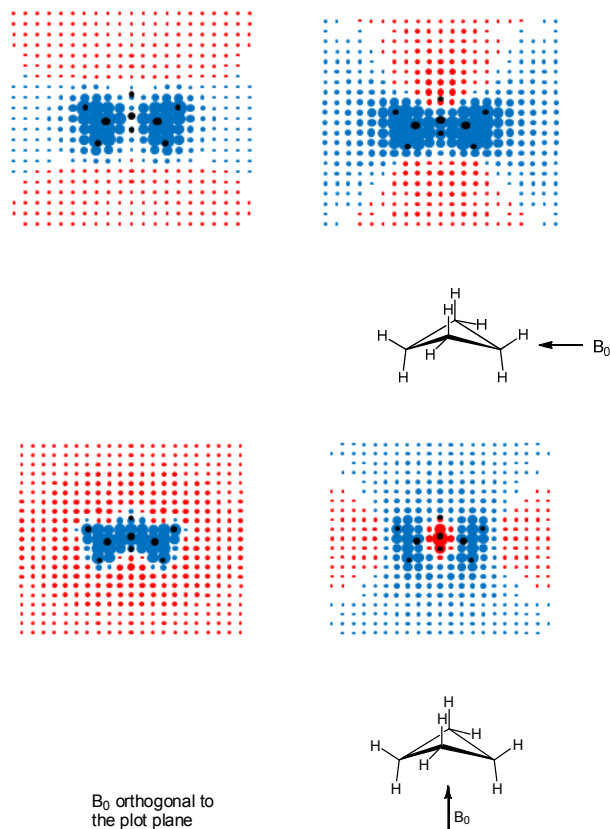


**Figure S1.** Visualization of total anisotropic effects of cyclopropane ( $D_{3h}$ ) in the  $\sigma_v$  plane: average of all space orientations (top left), when magnetic field is parallel to the  $C_2$  symmetry axis (top right), when magnetic field is orthogonal to the plot plane (bottom left), when magnetic field is orthogonal to the ring plane (bottom right). Blue and red points denote shielding and deshielding effects, respectively. The radius of points is proportional to the absolute value of the contribution. Positions of carbon and hydrogen nuclei are marked by black points.

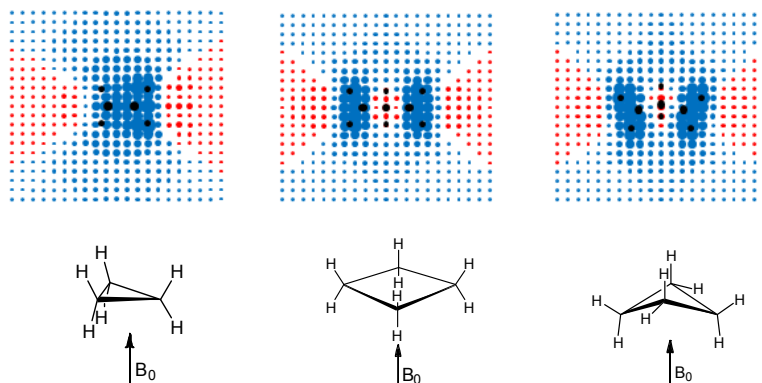




**Figure S2.** Visualization of (de)shielding contributions of cyclopentane ( $D_{5h}$ , upper part) and cyclohexane ( $D_{6h}$ , lower part) CC framework for a magnetic field applied perpendicularly to the ring plane: the first view is in the  $\sigma_v$  plane and the second view is in the plane of the carbon nuclei. The non-equivalence in the shielding pattern near the carbon nuclei, arising from the mismatch between the pentagonal/hexagonal molecule and square plotting grid is eliminated by the use of a finer grid, with a step width of 0.1 Å (right). Other details are the same as for Figure S1.



**Figure S3.** Visualization of total anisotropic effects of cyclobutane ( $D_{2d}$ ) in the  $\sigma_v$  plane, passing through the two  $\text{CH}_2$  groups: average of all space orientations (top left), when magnetic field is parallel to the  $C_1$  symmetry axis (top right), when magnetic field is orthogonal to the plot plane (bottom left), when magnetic field is parallel to the  $C_2$  symmetry axis (bottom right). Other details are the same as for Figure S1.



**Figure S4.** Visualization of (de)shielding contributions of C-H bonds of cyclopropane ( $D_{3h}$ ), left, cyclobutane ( $D_{4h}$ ), middle, and cyclobutane ( $D_{2d}$ ), right, for a magnetic field applied perpendicularly to the ring plane. The view is given in the  $\sigma_v$  planes. Other details are the same as for Figure S1.

## Evaluation of cyclopropane and cyclobutane strain energy

This was done at the same level used for the calculation of NMR parameters (B3LYP/6-311+G\*\*). The strain in the cyclopropane and cyclobutane was estimated as the difference in the total enthalpies and enthalpies of three and four CH<sub>2</sub> groups, respectively, where the enthalpy of CH<sub>2</sub> was calculated as the difference between propane and ethane (Table S7).

**Table S7.** Strain energies (kcal/mol) in cyclopropane and cyclobutane evaluated at the B3LYP/6-311+G\*\* level of theory.

Compound	Total Strain	
	exp <sup>a</sup>	calc
C <sub>3</sub> H <sub>6</sub>	27.5	24.5
C <sub>4</sub> H <sub>8</sub>	26.3	23.7
Difference C <sub>3</sub> H <sub>6</sub> – C <sub>4</sub> H <sub>8</sub>	1.2	0.8

<sup>a</sup> Taken from: Eliel, E. L.; Wilen, S. H.; Mander, L. N. *Stereochemistry of Organic Compounds*; John John Wiley and Sons, Inc, **1994**.

**Absolute energies (atomic units), x, y, z coordinates (Å) and vibrational frequencies  
of the optimized structures**

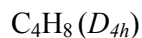
$C_3H_6(D_{3h})$

E = -117.930912 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.870969	0.000000
2	6	0	0.754281	-0.435485	0.000000
3	6	0	-0.754281	-0.435485	0.000000
4	1	0	0.000000	1.459331	0.909669
5	1	0	0.000000	1.459331	-0.909669
6	1	0	1.263818	-0.729666	0.909669
7	1	0	1.263818	-0.729666	-0.909669
8	1	0	-1.263818	-0.729666	-0.909669
9	1	0	-1.263818	-0.729666	0.909669

Vibrational frequencies ( $cm^{-1}$ ):

742.4485	742.4485	860.1183
877.9714	877.9714	1048.0976
1048.0976	1085.5896	1146.8648
1208.6255	1208.6255	1211.7934
1471.5978	1471.5978	1518.9107
3121.7961	3121.7961	3129.6787
3197.3274	3197.3274	3218.9472



E = -157.2558746 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.101720	0.000000
2	6	0	1.101720	0.000000	0.000000
3	6	0	0.000000	-1.101720	0.000000
4	6	0	-1.101720	0.000000	0.000000
5	1	0	0.000000	1.744401	0.883223
6	1	0	0.000000	1.744401	-0.883223
7	1	0	1.744401	0.000000	0.883223
8	1	0	1.744401	0.000000	-0.883223
9	1	0	0.000000	-1.744401	0.883223
10	1	0	0.000000	-1.744401	-0.883223
11	1	0	-1.744401	0.000000	0.883223
12	1	0	-1.744401	0.000000	-0.883223

Vibrational frequencies ( $cm^{-1}$ ):

-133.3899	738.3944	738.3944
742.2108	757.7007	910.9596
910.9596	969.0572	977.6521
999.3396	1152.4438	1226.4287
1232.8282	1250.5746	1250.5746
1264.7825	1283.8243	1283.8243
1479.7531	1483.6612	1483.6612
1519.3659	3040.1659	3043.5642
3043.5642	3055.7091	3066.4708
3086.8900	3086.8900	3108.6889

$C_4H_8(D_{2d})$ 

E = -157.2571529 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.084899	0.123544
2	6	0	-1.084899	0.000000	-0.123544
3	6	0	0.000000	-1.084899	0.123544
4	6	0	1.084899	0.000000	-0.123544
5	1	0	0.000000	1.960371	-0.528419
6	1	0	0.000000	1.425303	1.162127
7	1	0	-1.425303	0.000000	-1.162127
8	1	0	-1.960371	0.000000	0.528419
9	1	0	0.000000	-1.960371	-0.528419
10	1	0	0.000000	-1.425303	1.162127
11	1	0	1.425303	0.000000	-1.162127
12	1	0	1.960371	0.000000	0.528419

Vibrational frequencies ( $cm^{-1}$ ):

191.1690	639.0289	752.4690
752.4690	884.1020	911.6425
911.6425	940.5986	963.8172
1012.0724	1164.1154	1172.5608
1243.8251	1243.8251	1254.8956
1255.2700	1284.2238	1284.2238
1482.7991	1482.7991	1489.2568
1522.0069	3042.6571	3043.5887
3043.5887	3048.7119	3078.1866
3091.8175	3091.8175	3109.6722

$C_5H_{10}(D_{5h})$ 

E = -196.6047027 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.319635	0.000000
2	6	0	-1.255048	0.407790	0.000000
3	6	0	-0.775662	-1.067607	0.000000
4	6	0	0.775662	-1.067607	0.000000
5	6	0	1.255048	0.407790	0.000000
6	1	0	0.000000	1.976667	0.873566
7	1	0	-1.879922	0.610824	0.873566
8	1	0	-1.161856	-1.599157	0.873566
9	1	0	1.161856	-1.599157	0.873566
10	1	0	1.879922	0.610824	0.873566
11	1	0	1.161856	-1.599157	-0.873566
12	1	0	1.879922	0.610824	-0.873566
13	1	0	0.000000	1.976667	-0.873566
14	1	0	-1.879922	0.610824	-0.873566
15	1	0	-1.161856	-1.599157	-0.873566

Vibrational frequencies ( $cm^{-1}$ ):

-198.2665	-198.2665	688.5941
688.5941	730.9761	771.4599
771.4599	859.2343	917.3441
917.3441	1010.5691	1010.5691
1074.0028	1074.0028	1215.7588
1215.7588	1272.8051	1272.8051
1277.7828	1284.2105	1284.2105
1321.4716	1355.7643	1355.7643
1492.9864	1492.9864	1511.6940
1511.6940	1535.5268	3031.0027
3031.0027	3042.3628	3042.3628
3046.5029	3046.5029	3057.7659
3075.3969	3075.3969	3094.6573

$C_6H_{12}(D_{6h})$ 

E = -235.9044593 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.554601	0.000000
2	6	0	1.346324	0.777301	0.000000
3	6	0	1.346324	-0.777301	0.000000
4	6	0	0.000000	-1.554601	0.000000
5	6	0	-1.346324	-0.777301	0.000000
6	6	0	-1.346324	0.777301	0.000000
7	1	0	0.000000	2.220392	0.866672
8	1	0	1.922916	1.110196	-0.866672
9	1	0	1.922916	-1.110196	0.866672
10	1	0	0.000000	-2.220392	0.866672
11	1	0	-1.922916	-1.110196	0.866672
12	1	0	-1.922916	1.110196	0.866672
13	1	0	1.922916	1.110196	0.866672
14	1	0	1.922916	-1.110196	-0.866672
15	1	0	0.000000	-2.220392	-0.866672
16	1	0	-1.922916	-1.110196	-0.866672
17	1	0	-1.922916	1.110196	-0.866672
18	1	0	0.000000	2.220392	-0.866672

Vibrational frequencies ( $cm^{-1}$ ):

-347.8996	-238.5535	-238.5535
475.7533	475.7533	709.7189
729.3594	742.0399	742.0399
846.0444	858.9735	858.9735
945.6652	945.6652	1116.3846
1117.3499	1117.3499	1123.4835
1237.7751	1305.3238	1305.3238
1309.2148	1317.1000	1323.5001
1323.5001	1368.1422	1368.1422
1368.3454	1399.4176	1399.4176
1487.3348	1499.0265	1499.0265
1522.7514	1522.7514	1540.4520
3016.2396	3023.4505	3024.8359
3024.8359	3039.3759	3039.3759



3042.7853	3042.7853	3055.8255
3070.5287	3070.5287	3088.9283

**C<sub>6</sub>H<sub>12</sub> (*D*<sub>3d</sub>)**

E = -235.9448094 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.270269	0.733390	0.228186
2	6	0	0.000000	1.466780	-0.228186
3	6	0	1.270269	0.733390	0.228186
4	6	0	1.270269	-0.733390	-0.228186
5	6	0	0.000000	-1.466780	0.228186
6	6	0	-1.270269	-0.733390	-0.228186
7	1	0	2.160398	1.247306	-0.149994
8	1	0	0.000000	1.538437	-1.324085
9	1	0	0.000000	2.494613	0.149994
10	1	0	-1.332325	0.769218	1.324085
11	1	0	-2.160398	1.247306	-0.149994
12	1	0	1.332325	-0.769218	-1.324085
13	1	0	2.160398	-1.247306	0.149994
14	1	0	0.000000	-2.494613	-0.149994
15	1	0	0.000000	-1.538437	1.324085
16	1	0	-1.332325	-0.769218	-1.324085
17	1	0	-2.160398	-1.247306	0.149994
18	1	0	1.332325	0.769218	1.324085

**Vibrational frequencies (cm<sup>-1</sup>):**

228.9004	228.9004	376.5357
427.9887	427.9887	522.4859
427.9887	427.9887	522.4859
791.6736	791.6736	799.8103
862.6825	862.6825	917.1098
917.1098	1035.7014	1035.7014
1040.8734	1074.4892	1094.5788
1131.2112	1179.7913	1285.4803
1285.4803	1292.0092	1292.0092
1349.1099	1369.1718	1376.4482
1376.4482	1383.5299	1383.5299

1483.4829	1483.4829	1488.5623
1488.5623	1494.9184	1509.5691
2993.0594	2993.0594	2994.3155
3000.3654	3000.3654	3003.5069
3042.8680	3042.8680	3045.0991
3045.0991	3046.9691	3053.2751