

Supporting Information of

Systematic description of molecular formations with Cremer-Pople puckering and  
deformation coordinates utilizing analytic derivatives: applied to cycloheptane, cyclooctane,  
and cyclo[18]carbon

# Stationary Geometries

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Methods:

Cycloheptane: MP2/cc-pVTZ

Cyclooctane: MP2/cc-pVTZ except CC by MP2/6-311G and CCSD(T)/cc-pVTZ (Oct. 31, 2021)

Cyclo[18]carbon: M06-2X/def2-TZVPP

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# 1 Combinations of $(q_2, \phi_2)$ , $(q_3, \phi_3)$ , and $q_4$ at stationary points

Table S1: Cycloheptane ( $C_7H_{14}$ ). Unit:  $q_n$  in Å and  $\phi_n$  in Degree.<sup>a)</sup>

Form	Symm.			Form	Symm.		
		$q_2$	$q_3$			$q_2$	$q_3$
C	$C_s$	0.460	0.658	TC	$C_2$	0.547	0.649
BTS	$C_s$	0.914	0.302	TTS	$C_2$	1.015	0.304
B	$C_s$	1.173	0.015	TB	$C_2$	1.172	0.012
		$\phi_2$	$\phi_3$			$\phi_2$	$\phi_3$
		0.0	180.0			38.6	192.9
		77.1	205.7			115.7	218.6
		154.3	231.4			192.9	244.3
		231.4	257.1			270.0	270.0
		308.6	282.9			347.1	295.7
		385.7 (= 25.7)	308.6			424.3 (= 64.3)	321.4
		462.9 (=102.9)	334.3			501.4 (=141.4)	347.1
		540.0 (=180.0)	360.0 (= 0.0)			578.6 (=218.6)	372.9 (= 12.9)
		617.1 (=257.1)	385.7 (= 25.7)			655.7 (=295.7)	398.6 (= 38.6)
		694.3 (=334.3)	411.4 (= 51.4)			732.9 (= 12.9)	424.3 (= 64.3)
		771.4 (= 51.4)	437.1 (= 77.1)			810.0 (= 90.0)	450.0 (= 90.0)
		848.6 (=128.6)	462.9 (=102.9)			887.1 (=167.1)	475.7 (=115.7)
		925.7 (=205.7)	488.6 (=128.6)			964.3 (=244.3)	501.4 (=141.4)
		1002.9 (=282.9)	514.3 (=154.3)			1041.4 (=321.4)	527.1 (=167.1)

<sup>a)</sup> The general formula for  $\{\phi_2, \phi_3\}$  is  $\{3m\pi/7, \pi + m\pi/7\}$  at  $C_s$  geometries and  $\{3(m + \frac{1}{2})\pi/7, \pi + (m + \frac{1}{2})\pi/7\}$  at  $C_2$  (in radians), where  $m = 0, 1, \dots, 13$ .

Table S2: Cyclooctane ( $C_8H_{16}$ ). Unit:  $q_n$  in Å and  $\phi_n$  in Degree.

Form	Symm.	$(q_2, \phi_2)$	$(q_3, \phi_3)$	$q_4$	Form	Symm.	$(q_2, \phi_2)$	$(q_3, \phi_3)$	$q_4$
CR	$D_{4d}$	0.000	0.000	0.808					
		0.0	0.0						
CC	$C_{2v}$	0.225	0.000	0.836	NT7	$D_2$	0.202	0.000	0.806
NT3	$C_{2v}$	1.143	0.000	0.324	TCC	$D_2$	0.434	0.000	0.790
BB	$D_{2d}$	1.518	0.000	0.000	NT5	$D_2$	1.396	0.000	0.316
					TB	$D_2$	1.630	0.000	0.107
					B	$D_{2d}$	1.648	0.000	0.000
		0.0	0.0				45.0	0.0	
		90.0	0.0				135.0	0.0	
		180.0	0.0				225.0	0.0	
		270.0	0.0				315.0	0.0	
TCC	$C_{2h}$	0.000	0.953	0.000	C	$C_{2h}$	0.000	0.944	0.000
		0.0	0.0				0.0	22.5	
		0.0	135.0				0.0	157.5	
		0.0	270.0				0.0	292.5	
		0.0	45.0				0.0	67.5	
		0.0	180.0				0.0	202.5	
		0.0	315.0				0.0	337.5	
		0.0	90.0				0.0	112.5	
		0.0	225.0				0.0	247.5	
NT2	$C_s$	0.385	0.876	0.180	TBC	$C_2$	0.720	0.833	0.220
NT4	$C_s$	0.767	0.338	0.562	WT1	$C_2$	1.138	0.274	0.449
BC	$C_s$	1.052	0.587	0.345	NT6	$C_2$	1.519	0.125	0.208
WT4	$C_s$	1.420	0.243	0.139					
		0.0	0.0 <sup>a)</sup>				45.0	112.5 <sup>a)</sup>	
		90.0	135.0 <sup>a)</sup>				135.0	247.5 <sup>a)</sup>	
		180.0	270.0 <sup>a)</sup>				225.0	22.5 <sup>a)</sup>	
		270.0	45.0 <sup>a)</sup>				315.0	157.5 <sup>a)</sup>	
		0.0	180.0 <sup>a)</sup>				45.0	292.5 <sup>a)</sup>	
		90.0	315.0 <sup>a)</sup>				135.0	67.5 <sup>a)</sup>	
		180.0	90.0 <sup>a)</sup>				225.0	202.5 <sup>a)</sup>	
		270.0	225.0 <sup>a)</sup>				315.0	337.5 <sup>a)</sup>	
S	$S_4$	1.595	0.000	0.000	NT1	$C_2$	1.134	0.500	0.000
		18.5	0.0				0.0	135.0 <sup>a)</sup>	
		108.5	0.0				90.0	270.0 <sup>a)</sup>	
		198.5	0.0				180.0	45.0 <sup>a)</sup>	
		288.5	0.0				270.0	180.0 <sup>a)</sup>	
		71.5 <sup>b)</sup>	0.0				0.0	315.0 <sup>a)</sup>	
		161.5 <sup>b)</sup>	0.0				90.0	90.0 <sup>a)</sup>	
		251.5 <sup>b)</sup>	0.0				180.0	225.0 <sup>a)</sup>	
		341.5 <sup>b)</sup>	0.0				270.0	0.0 <sup>a)</sup>	
WT2	$C_1$	0.907	0.719	0.276	WT2 <sup>b)</sup>	$C_1$	0.907	0.719	0.276
		66.27	117.97 <sup>a)</sup>				23.73	107.03 <sup>a)</sup>	
		156.27	252.97 <sup>a)</sup>				113.73	242.03 <sup>a)</sup>	
		246.27	27.97 <sup>a)</sup>				203.73	17.03 <sup>a)</sup>	
		336.27	162.97 <sup>a)</sup>				293.73	152.03 <sup>a)</sup>	
		66.27	297.97 <sup>a)</sup>				23.73	287.03 <sup>a)</sup>	
		156.27	72.97 <sup>a)</sup>				113.73	62.03 <sup>a)</sup>	
		246.27	207.97 <sup>a)</sup>				203.73	197.03 <sup>a)</sup>	
		336.27	342.97 <sup>a)</sup>				293.73	332.03 <sup>a)</sup>	

<sup>a)</sup> After inversion operation of Cartesian coordinates,  $\phi_3$  is shifted by  $-90^\circ$ .

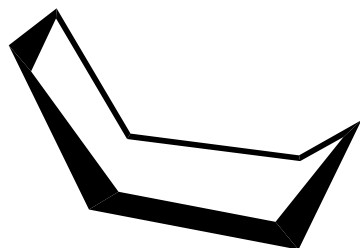
<sup>b)</sup> Atoms are ordered counterclockwise.

## 2 Cycloheptane (C<sub>7</sub>H<sub>14</sub>)

### 2.1 C<sub>7</sub>H<sub>14</sub>: Boat / B / C<sub>s</sub>

Puckering coordinates			
	q	phi	theta
2.	1.17263	0.00000	89.25618
3.	0.01522	180.00000	
Planar coordinates			
	t	tau	gamma
1.	0.00656	0.00000	3.12675
2.	0.00227	0.00000	1.08449
3.	0.11699	0.00000	77.11039
4.	0.02444	0.00000	65.93574
5.	0.01092	0.00000	0.00000
R	1.55370		

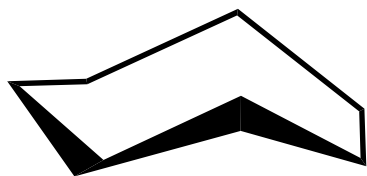
C	1.41250043	-0.57151722	-0.00000000
C	0.65324395	-0.86691242	1.29047522
C	-0.68126437	-0.11876576	1.42793768
C	-0.68126437	1.26413142	0.77671280
C	-0.68126437	1.26413142	-0.77671280
C	-0.68126437	-0.11876576	-1.42793768
C	0.65324395	-0.86691242	-1.29047522
H	1.29902061	-0.59019605	2.12678737
H	1.29902061	-0.59019605	-2.12678737
H	0.48092211	-1.94197175	1.37930498
H	0.48092211	-1.94197175	-1.37930498
H	1.70885538	0.47969724	-0.00000000
H	2.34365962	-1.14188368	-0.00000000
H	-0.91458828	-0.00771487	-2.48821668
H	-0.91458828	-0.00771487	2.48821668
H	-1.49212268	-0.71465006	-1.01026272
H	-1.49212268	-0.71465006	1.01026272
H	0.17961635	1.82457635	-1.14702303
H	0.17961635	1.82457635	1.14702303
H	-1.56089819	1.80488177	-1.12751452
H	-1.56089819	1.80488177	1.12751452



## 2.2 C<sub>7</sub>H<sub>14</sub>: Chair / C / C<sub>s</sub>

Puckering coordinates			
	q	phi	theta
2.	0.45991	180.00000	34.96117
3.	0.65777	0.00000	
Planar coordinates			
	t	tau	gamma
1.	0.00354	180.00000	2.40786
2.	0.06944	180.00000	55.47833
3.	0.01982	0.00000	24.51668
4.	0.00121	0.00000	1.60019
5.	0.04344	180.00000	0.00000
R	1.63387		

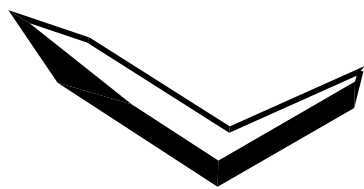
C	-0.76606605	1.55537811	-0.00000000
C	-0.72390005	0.74018805	-1.28681209
C	0.55356304	-0.07888901	-1.47869311
C	0.55356304	-1.43380010	-0.77336605
C	0.55356304	-1.43380010	0.77336605
C	0.55356304	-0.07888901	1.47869311
C	-0.72390005	0.74018805	1.28681209
H	0.68640305	-0.27286302	-2.54499818
H	0.68640305	-0.27286302	2.54499818
H	1.41799410	0.51523704	-1.17121008
H	1.41799410	0.51523704	1.17121008
H	-0.31484202	-1.98859914	-1.13448408
H	-0.31484202	-1.98859914	1.13448408
H	1.42402510	-1.99204814	-1.12095208
H	1.42402510	-1.99204814	1.12095208
H	-0.83265906	1.42873510	2.12718616
H	-0.83265906	1.42873510	-2.12718616
H	-1.58729511	0.06855001	1.32598210
H	-1.58729511	0.06855001	-1.32598210
H	-1.66909412	2.16978016	-0.00000000
H	0.07952101	2.24993016	-0.00000000



### 2.3 C<sub>7</sub>H<sub>14</sub>: Bent transition state / BTS / C<sub>s</sub>

Puckering coordinates			
	q	phi	theta
2.	0.91415	0.00000	71.73801
3.	0.30165	180.00000	
Planar coordinates			
	t	tau	gamma
1.	0.05178	180.00000	27.52607
2.	0.07019	180.00000	44.94487
3.	0.06391	0.00000	65.34405
4.	0.01114	0.00000	22.32369
5.	0.02714	180.00000	0.00000
R	1.62076		

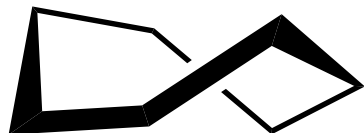
C	-0.52777448	1.63871192	0.00000000
C	-0.15589635	0.99722651	1.36546902
C	0.58936473	-0.33394389	1.42152292
C	-0.15589635	-1.49489646	0.77298751
C	-0.15589635	-1.49489646	-0.77298751
C	0.58936473	-0.33394389	-1.42152292
C	-0.15589635	0.99722651	-1.36546902
H	-0.11110533	2.64507369	-0.00000000
H	-1.60686237	1.78794829	0.00000000
H	0.28493555	-2.42808201	1.12539196
H	-1.18165461	-1.48973352	1.14756768
H	0.28493555	-2.42808201	-1.12539196
H	-1.18165461	-1.48973352	-1.14756768
H	0.42763501	1.72350038	1.93322262
H	-1.07847585	0.85940200	1.93349654
H	0.42763501	1.72350038	-1.93322262
H	-1.07847585	0.85940200	-1.93349654
H	1.59128824	-0.23872633	1.00316008
H	0.73314677	-0.56932417	2.47858172
H	1.59128824	-0.23872633	-1.00316008
H	0.73314677	-0.56932417	-2.47858172



## 2.4 C<sub>7</sub>H<sub>14</sub>: Twist boat / TB / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.17226	270.00000	89.40792
3.	0.01211	90.00000	
Planar coordinates			
	t	tau	gamma
1.	0.00684	0.00000	3.25982
2.	0.00073	180.00000	0.34712
3.	0.11699	180.00000	77.02316
4.	0.02454	180.00000	65.55167
5.	0.01116	180.00000	0.00000
R	1.55387		

C	0.00000000	-0.00000000	1.70142974
C	-1.19325661	-0.46017254	0.86675393
C	-0.84231150	-1.39611494	-0.28983248
C	-0.00000000	-0.76371031	-1.42422739
C	-0.00000000	0.76371031	-1.42422739
C	0.84231150	1.39611494	-0.28983248
C	1.19325661	0.46017254	0.86675393
H	0.32863946	2.27640845	0.10341660
H	-0.32863946	-2.27640845	0.10341660
H	1.77976573	1.75957923	-0.71404982
H	-1.77976573	-1.75957923	-0.71404982
H	-1.03001505	1.11796088	-1.37454708
H	1.03001505	-1.11796088	-1.37454708
H	0.38527879	1.11351300	-2.38282099
H	-0.38527879	-1.11351300	-2.38282099
H	1.71484075	-0.41325963	0.47288142
H	-1.71484075	0.41325963	0.47288142
H	-1.90999538	-0.96292550	1.51906073
H	1.90999538	0.96292550	1.51906073
H	-0.32210842	0.81359020	2.35560558
H	0.32210842	-0.81359020	2.35560558





2.5 C<sub>7</sub>H<sub>14</sub>: Twist chair / TC / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	0.54725	270.00000	40.14233
3.	0.64890	270.00000	
Planar coordinates			
	t	tau	gamma
1.	0.01904	0.00000	11.08164
2.	0.07741	180.00000	52.78946
3.	0.02569	180.00000	25.91925
4.	0.01132	180.00000	12.36397
5.	0.05164	180.00000	0.00000
R	1.62063		

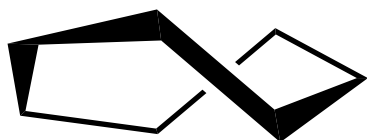
C	0.00000000	-0.00000000	1.76834513
C	0.00000000	1.29501509	0.95216407
C	-0.88033706	1.28088409	-0.30018602
C	-0.15089301	0.74773205	-1.53372011
C	0.15089301	-0.74773205	-1.53372011
C	0.88033706	-1.28088409	-0.30018602
C	-0.00000000	-1.29501509	0.95216407
H	-0.30808902	2.10835815	1.61108611
H	0.30808902	-2.10835815	1.61108611
H	1.02044707	1.53345511	0.64283905
H	-1.02044707	-1.53345511	0.64283905
H	0.87265206	0.00909200	2.42487218
H	-0.87265206	-0.00909200	2.42487218
H	1.79287813	-0.70570105	-0.11913501
H	-1.79287813	0.70570105	-0.11913501
H	1.20079008	-2.30158716	-0.51584904
H	-1.20079008	2.30158716	-0.51584904
H	0.73635205	-0.97772807	-2.42661417
H	-0.73635205	0.97772807	-2.42661417
H	-0.78766706	-1.30129510	-1.63178512
H	0.78766706	1.30129510	-1.63178512



2.6 C<sub>7</sub>H<sub>14</sub>: Twist transition state / TTS / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.01450	90.00000	73.33881
3.	0.30362	90.00000	
Planar coordinates			
	t	tau	gamma
1.	0.06654	0.00000	29.08874
2.	0.07556	180.00000	39.18181
3.	0.08006	180.00000	59.72136
4.	0.01877	180.00000	23.67656
5.	0.04281	180.00000	0.00000
R	1.58413		

C	0.00000000	0.00000000	1.74007108
C	-0.94565522	0.84787892	0.89007285
C	-0.18683690	1.57408977	-0.21668968
C	0.00000000	0.77786820	-1.52496277
C	-0.00000000	-0.77786820	-1.52496277
C	0.18683690	-1.57408977	-0.21668968
C	0.94565522	-0.84787892	0.89007285
H	-0.78952850	1.08441284	-2.21172871
H	0.78952850	-1.08441284	-2.21172871
H	0.92653222	1.12191106	-1.98576410
H	-0.92653222	-1.12191106	-1.98576410
H	0.78622680	1.87226113	0.17985455
H	-0.78622680	-1.87226113	0.17985455
H	-0.69862795	2.50329652	-0.46943635
H	0.69862795	-2.50329652	-0.46943635
H	1.72678922	-0.22290460	0.45165727
H	-1.72678922	0.22290460	0.45165727
H	-1.45481572	1.56692258	1.53327213
H	1.45481572	-1.56692258	1.53327213
H	0.57991301	0.65786319	2.39140952
H	-0.57991301	-0.65786319	2.39140952



2.7  $C_7H_{14}$ : Plane / P /  $D_{7h}$

Puckering coordinates			
	q	phi	theta
2.	0.00000	0.00000	90.00000
3.	0.00000	0.00000	
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.00000	0.00000	0.00000
5.	0.00000	0.00000	0.00000
R	1.78885		

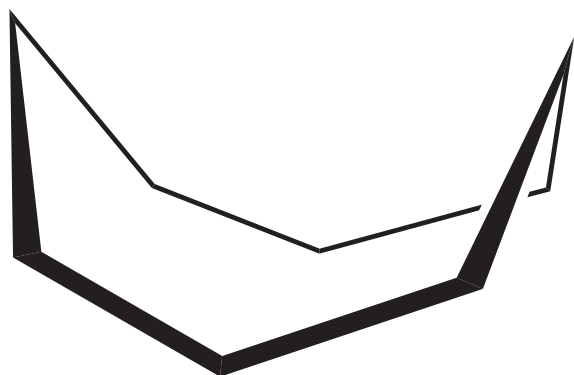
C	-0.00000000	1.78884913	-0.00000000
C	-1.39857862	1.11532916	-0.00000000
C	-1.74399901	-0.39805647	-0.00000000
C	-0.77615258	-1.61169751	-0.00000000
C	0.77615258	-1.61169751	-0.00000000
C	1.74399901	-0.39805647	-0.00000000
C	1.39857862	1.11532916	-0.00000000
H	-0.00000000	2.45833318	0.85911506
H	-1.92200233	1.53274564	0.85911506
H	-2.39669770	-0.54703068	0.85911506
H	-1.06663082	-2.21488180	0.85911506
H	1.06663082	-2.21488180	0.85911506
H	2.39669770	-0.54703068	0.85911506
H	1.92200233	1.53274564	0.85911506
H	0.00000000	2.45833318	-0.85911506
H	-1.92200233	1.53274564	-0.85911506
H	-2.39669770	-0.54703068	-0.85911506
H	-1.06663082	-2.21488180	-0.85911506
H	1.06663082	-2.21488180	-0.85911506
H	2.39669770	-0.54703068	-0.85911506
H	1.92200233	1.53274564	-0.85911506

### 3 Cyclooctane (C<sub>8</sub>H<sub>16</sub>)

#### 3.1 C<sub>8</sub>H<sub>16</sub>: Boat-boat / BB / D<sub>2d</sub>

Puckering coordinates			
	q	phi	theta
2.	1.51831	0.00000	90.00000
3.	0.00000	0.00000	90.00000
4.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.16598	0.00000	90.00000
5.	0.00000	0.00000	0.00000
6.	0.00000	0.00000	0.00000
R	1.69305		

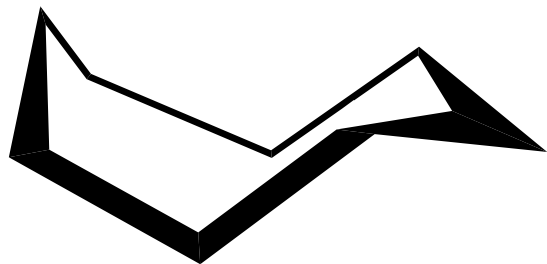
C	0.00000000	1.52707376	0.75915687
C	1.31453275	1.31453275	-0.00000000
C	1.52707376	-0.00000000	-0.75915687
C	1.31453275	-1.31453275	-0.00000000
C	-0.00000000	-1.52707376	0.75915687
C	-1.31453275	-1.31453275	-0.00000000
C	-1.52707376	0.00000000	-0.75915687
C	-1.31453275	1.31453275	-0.00000000
H	0.00000000	2.56143973	1.11281550
H	0.00000000	0.92329247	1.66225510
H	-0.00000000	-2.56143973	1.11281550
H	-0.00000000	-0.92329247	1.66225510
H	0.92329247	-0.00000000	-1.66225510
H	2.56143973	-0.00000000	-1.11281550
H	-0.92329247	0.00000000	-1.66225510
H	-2.56143973	0.00000000	-1.11281550
H	1.43520740	2.12747368	-0.72154851
H	2.12747368	1.43520740	0.72154851
H	1.43520740	-2.12747368	-0.72154851
H	2.12747368	-1.43520740	0.72154851
H	-1.43520740	-2.12747368	-0.72154851
H	-2.12747368	-1.43520740	0.72154851
H	-1.43520740	2.12747368	-0.72154851
H	-2.12747368	1.43520740	0.72154851



### 3.2 C<sub>8</sub>H<sub>16</sub>: Boat-chair / BC / C<sub>s</sub>

Puckering coordinates			
	q	phi	theta
2.	1.05153	0.00000	57.06892
3.	0.58724	0.00000	120.43228
4.	-0.34498		
Planar coordinates			
	t	tau	gamma
1.	0.04705	0.00000	17.56644
2.	0.04867	180.00000	19.11445
3.	0.10313	0.00000	47.24785
4.	0.08300	0.00000	60.53487
5.	0.03832	0.00000	54.80950
6.	0.02703	180.00000	0.00000
R	1.74298		

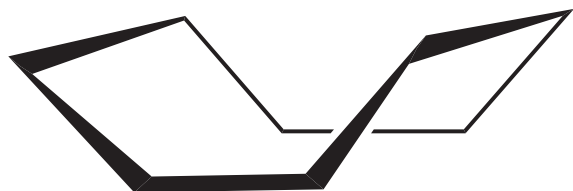
C	-0.93612121	1.41640016	-0.00000000
C	-0.13620177	1.37617687	1.29774348
C	0.64292226	0.08785809	1.58427924
C	-0.13620177	-1.20911021	1.31520338
C	0.20105905	-1.91555650	0.00000000
C	-0.13620177	-1.20911021	-1.31520338
C	0.64292226	0.08785809	-1.58427924
C	-0.13620177	1.37617687	-1.29774348
H	-1.52547964	2.33613073	-0.00000000
H	-1.66584300	0.60457084	-0.00000000
H	1.27384554	-2.13255376	0.00000000
H	-0.30312640	-2.88498492	0.00000000
H	1.57508445	0.07097581	1.02015431
H	0.93821856	0.11640061	2.63437677
H	1.57508445	0.07097581	-1.02015431
H	0.93821856	0.11640061	-2.63437677
H	0.55181222	2.22550158	1.32403532
H	-0.83971526	1.52961148	2.12018752
H	0.07794163	-1.91867679	2.11629323
H	-1.21096562	-1.01747363	1.37066363
H	0.07794163	-1.91867679	-2.11629323
H	-1.21096562	-1.01747363	-1.37066363
H	0.55181222	2.22550158	-1.32403532
H	-0.83971526	1.52961148	-2.12018752



### 3.3 C<sub>8</sub>H<sub>16</sub>: Boat / B / D<sub>2d</sub>

Puckering coordinates			
	q	phi	theta
2.	1.64779	45.00000	90.00000
3.	0.00000	0.00000	90.00000
4.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.15127	90.00000	90.00000
5.	0.00000	0.00000	0.00000
6.	0.00000	0.00000	0.00000
R	1.65965		

C	0.77487303	1.47542446	0.58258193
C	1.47542446	0.77487303	-0.58258193
C	1.47542446	-0.77487303	-0.58258193
C	0.77487303	-1.47542446	0.58258193
C	-0.77487303	-1.47542446	0.58258193
C	-1.47542446	-0.77487303	-0.58258193
C	-1.47542446	0.77487303	-0.58258193
C	-0.77487303	1.47542446	0.58258193
H	1.14546306	1.06287249	1.52099048
H	1.11133370	2.51318592	0.57390295
H	-1.14546306	-1.06287249	1.52099048
H	-1.11133370	-2.51318592	0.57390295
H	2.51318592	-1.11133370	-0.57390295
H	1.06287249	-1.14546306	-1.52099048
H	-2.51318592	1.11133370	-0.57390295
H	-1.06287249	1.14546306	-1.52099048
H	2.51318592	1.11133370	-0.57390295
H	1.06287249	1.14546306	-1.52099048
H	1.14546306	-1.06287249	1.52099048
H	1.11133370	-2.51318592	0.57390295
H	-2.51318592	-1.11133370	-0.57390295
H	-1.06287249	-1.14546306	-1.52099048
H	-1.14546306	1.06287249	1.52099048
H	-1.11133370	2.51318592	0.57390295



### 3.4 C<sub>8</sub>H<sub>16</sub>: Chair / C / C<sub>2h</sub>

Puckering coordinates			
	q	phi	theta
2.	0.00000	0.00000	0.00000
3.	0.94360	22.50000	90.00000
4.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.13597	45.00000	42.93164
3.	0.00000	0.00000	0.00000
4.	0.01641	270.00000	6.44635
5.	0.00000	0.00000	0.00000
6.	0.14524	315.00000	0.00000
R	1.80427		

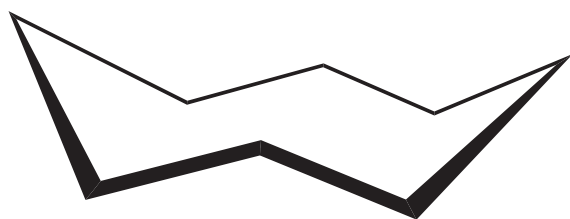
C	-1.15183768	1.11880601	0.43525905
C	0.02335668	1.60558705	-0.43525929
C	1.40927616	1.42331457	0.18236490
C	2.00294464	-0.00992652	0.18236431
C	1.15183768	-1.11880601	-0.43525905
C	-0.02335668	-1.60558705	0.43525929
C	-1.40927616	-1.42331457	-0.18236490
C	-2.00294464	0.00992652	-0.18236431
H	-2.24920322	0.30742520	-1.20346041
H	-2.95410557	-0.01883106	0.35115891
H	2.95410557	0.01883106	-0.35115891
H	2.24920322	-0.30742520	1.20346041
H	-0.01700241	1.12640722	-1.41527653
H	-0.10630569	2.67156358	-0.62938941
H	0.10630569	-2.67156358	0.62938941
H	0.01700241	-1.12640722	1.41527653
H	-1.81391172	1.96425058	0.62938849
H	-0.78446837	0.80851357	1.41527656
H	2.10218319	2.07555331	-0.35115699
H	1.37304277	1.80780786	1.20346140
H	0.78446837	-0.80851357	-1.41527656
H	1.81391172	-1.96425058	-0.62938849
H	-1.37304277	-1.80780786	-1.20346140
H	-2.10218319	-2.07555331	0.35115699



### 3.5 C<sub>8</sub>H<sub>16</sub>: Crown / CR / D<sub>4d</sub>

Puckering coordinates			
	q	phi	theta
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.80812		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.00000	0.00000	0.00000
5.	0.00000	0.00000	0.00000
6.	0.00000	0.00000	0.00000
R	1.85268		

C	0.00000000	1.85268133	0.28571256
C	1.31004353	1.31004353	-0.28571256
C	1.85268133	-0.00000000	0.28571256
C	1.31004353	-1.31004353	-0.28571256
C	-0.00000000	-1.85268133	0.28571256
C	-1.31004353	-1.31004353	-0.28571256
C	-1.85268133	0.00000000	0.28571256
C	-1.31004353	1.31004353	-0.28571256
H	0.00000000	2.93021446	0.10815758
H	0.00000000	1.73030774	1.37347715
H	-0.00000000	-2.93021446	0.10815758
H	-0.00000000	-1.73030774	1.37347715
H	2.93021446	-0.00000000	0.10815758
H	1.73030774	-0.00000000	1.37347715
H	-2.93021446	0.00000000	0.10815758
H	-1.73030774	0.00000000	1.37347715
H	1.22351234	1.22351234	-1.37347715
H	2.07197452	2.07197452	-0.10815758
H	1.22351234	-1.22351234	-1.37347715
H	2.07197452	-2.07197452	-0.10815758
H	-1.22351234	-1.22351234	-1.37347715
H	-2.07197452	-2.07197452	-0.10815758
H	-1.22351234	1.22351234	-1.37347715
H	-2.07197452	2.07197452	-0.10815758

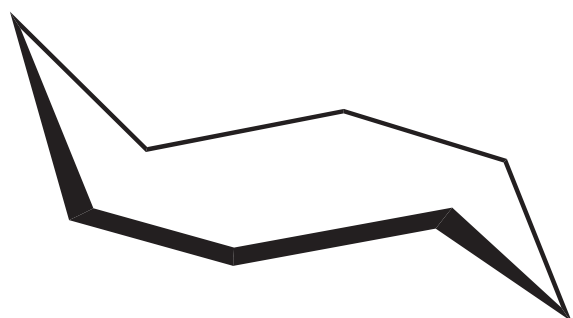




### 3.6 C<sub>8</sub>H<sub>16</sub>: Twist chair / TC / C<sub>2h</sub>

Puckering coordinates			
	q	phi	theta
2.	0.00000	0.00000	0.00000
3.	0.95326	0.00000	90.00000
4.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.13774	0.00000	41.11161
3.	0.00000	0.00000	0.00000
4.	0.00122	0.00000	0.44262
5.	0.00000	0.00000	0.00000
6.	0.15782	0.00000	0.00000
R	1.79980		

C	-0.84900245	1.32869724	0.00000000
C	-0.00000000	1.30362884	1.28771348
C	-0.00000000	0.00000000	2.09413861
C	-0.00000000	-1.30362884	1.28771348
C	0.84900245	-1.32869724	-0.00000000
C	0.00000000	-1.30362884	-1.28771348
C	-0.00000000	-0.00000000	-2.09413861
C	0.00000000	1.30362884	-1.28771348
H	-1.45126989	2.23662170	0.00000000
H	-1.56310598	0.50276426	0.00000000
H	1.56310598	-0.50276426	-0.00000000
H	1.45126989	-2.23662170	0.00000000
H	0.87112492	0.01845475	2.75267933
H	-0.87112492	-0.01845475	2.75267933
H	0.87112492	0.01845475	-2.75267933
H	-0.87112492	-0.01845475	-2.75267933
H	1.02754028	1.55369500	1.01897684
H	-0.32402468	2.10134907	1.95772764
H	0.32402468	-2.10134907	1.95772764
H	-1.02754028	-1.55369500	1.01897684
H	0.32402468	-2.10134907	-1.95772764
H	-1.02754028	-1.55369500	-1.01897684
H	1.02754028	1.55369500	-1.01897684
H	-0.32402468	2.10134907	-1.95772764



### 3.7 C<sub>8</sub>H<sub>16</sub>: Chair-chair / CC / C<sub>2v</sub>

MP2/6-311G results

```

      Puckering coordinates
            q      phi      theta
2.      0.22490    0.00000    15.05376
3.      0.00000    0.00000    0.00000
4.      0.83620
      Planar coordinates
            t      tau      gamma
1.      0.00000    0.00000    0.00000
2.      0.05780    0.00000    43.97353
3.      0.00000    0.00000    0.00000
4.      0.00500    0.00000    4.78748
5.      0.00000    0.00000    0.00000
6.      0.05970    0.00000    0.00000
R      1.85850

```

C	0.00000000	1.73600013	0.40834584
C	1.31903710	1.31635010	-0.29538621
C	1.97100015	-0.00000000	0.18344583
C	1.31903710	-1.31635010	-0.29538621
C	-0.00000000	-1.73600013	0.40834584
C	-1.31903710	-1.31635010	-0.29538621
C	-1.97100015	0.00000000	0.18344583
C	-1.31903710	1.31635010	-0.29538621
H	3.01332823	-0.00000000	-0.16992720
H	2.01045515	-0.00000000	1.28453991
H	-2.01045515	0.00000000	1.28453991
H	-3.01332823	0.00000000	-0.16992720
H	1.14768809	-1.25453110	-1.38182129
H	2.05643516	-2.11759616	-0.14108520
H	1.14768809	1.25453110	-1.38182129
H	2.05643516	2.11759616	-0.14108520
H	0.00000000	-1.35538410	1.44167692
H	0.00000000	-2.83253422	0.48340785
H	0.00000000	1.35538410	1.44167692
H	0.00000000	2.83253422	0.48340785
H	-1.14768809	-1.25453110	-1.38182129
H	-2.05643516	-2.11759616	-0.14108520
H	-1.14768809	1.25453110	-1.38182129
H	-2.05643516	2.11759616	-0.14108520

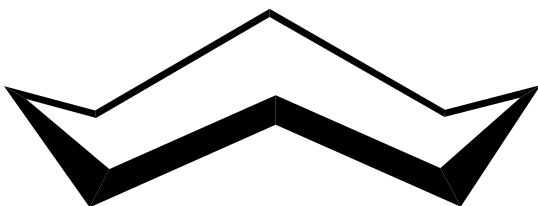
CCSD(T)/cc-pVTZ results

```

      Puckering coordinates
            q      phi      theta
2.      0.00550   180.00000    0.38759
3.      0.00000    0.00000    0.00000
4.      0.81296
      Planar coordinates
            t      tau      gamma
1.      0.00000    0.00000    0.00000
2.      0.00129   180.00000    48.01121
3.      0.00000    0.00000    0.00000
4.      0.00005    0.00000    2.31486
5.      0.00000    0.00000    0.00000
6.      0.00116   180.00000    0.00000
R      1.85979

```

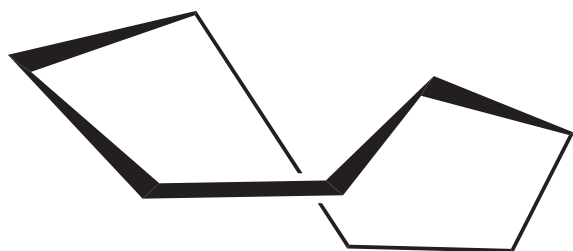
C	1.86218884	0.00000000	0.28466295
C	1.31500923	-1.31519282	-0.28743903
C	0.00000000	-1.85729108	0.29016250
C	-1.31500923	-1.31519282	-0.28743903
C	-1.86218884	0.00000000	0.28466295
C	-1.31500923	1.31519282	-0.28743903
C	0.00000000	1.85729108	0.29016250
C	1.31500923	1.31519282	-0.28743903
H	0.00000000	-2.93843225	0.11766755
H	0.00000000	2.93843225	0.11766755
H	0.00000000	-1.72761792	1.37984184
H	0.00000000	1.72761792	1.37984184
H	-1.22559599	-1.22887601	-1.37775570
H	1.22559599	-1.22887601	-1.37775570
H	-1.22559599	1.22887601	-1.37775570
H	1.22559599	1.22887601	-1.37775570
H	-2.07833078	-2.07953290	-0.10947845
H	2.07833078	-2.07953290	-0.10947845
H	-2.07833078	2.07953290	-0.10947845
H	2.07833078	2.07953290	-0.10947845
H	-1.74240774	0.00000000	1.37542554
H	1.74240774	0.00000000	1.37542554
H	-2.94166724	0.00000000	0.10215981
H	2.94166724	0.00000000	0.10215981



### 3.8 C<sub>8</sub>H<sub>16</sub>: Twist boat / TB / D<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.63000	45.00000	86.25072
3.	0.00000	0.00000	0.00000
4.	0.10682		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.07643	45.00000	25.61789
3.	0.00000	0.00000	0.00000
4.	0.14286	90.00000	63.68227
5.	0.00000	0.00000	0.00000
6.	0.07066	315.00000	0.00000
R	1.65728		

C	-0.45865892	1.49127112	0.61405621
C	0.45865892	1.49127112	-0.61405621
C	1.68033295	0.54579183	-0.53852658
C	1.68033295	-0.54579183	0.53852658
C	0.45865892	-1.49127112	0.61405621
C	-0.45865892	-1.49127112	-0.61405621
C	-1.68033295	-0.54579183	-0.53852658
C	-1.68033295	0.54579183	0.53852658
H	2.57518457	-1.14524854	0.36129392
H	1.83398480	-0.08520331	1.51504138
H	1.83398480	0.08520331	-1.51504138
H	2.57518457	1.14524854	-0.36129392
H	-2.57518457	1.14524854	0.36129392
H	-1.83398480	0.08520331	1.51504138
H	-1.83398480	-0.08520331	-1.51504138
H	-2.57518457	-1.14524854	-0.36129392
H	-0.13322331	1.25961663	-1.49909840
H	0.83103712	2.50333219	-0.77332392
H	-0.83103712	2.50333219	0.77332392
H	0.13322331	1.25961663	1.49909840
H	0.13322331	-1.25961663	-1.49909840
H	-0.83103712	-2.50333219	-0.77332392
H	0.83103712	-2.50333219	0.77332392
H	-0.13322331	-1.25961663	1.49909840



### 3.9 C<sub>8</sub>H<sub>16</sub>: Twist chair-chair / TCC / D<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	0.43444	315.00000	28.80659
3.	0.00000	0.00000	0.00000
4.	0.79004		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.10837	315.00000	43.77258
3.	0.00000	0.00000	0.00000
4.	0.00114	270.00000	0.57680
5.	0.00000	0.00000	0.00000
6.	0.11311	45.00000	0.00000
R	1.81921		

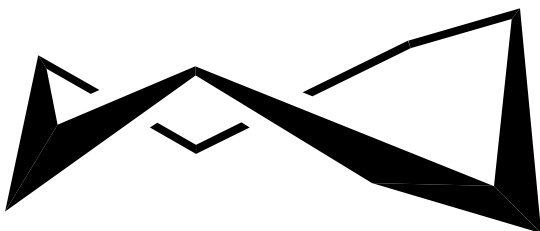
C	0.63829200	1.53519068	0.43291982
C	1.82714347	0.75196722	-0.12572088
C	1.82714347	-0.75196722	0.12572088
C	0.63829200	-1.53519068	-0.43291982
C	-0.63829200	-1.53519068	0.43291982
C	-1.82714347	-0.75196722	-0.12572088
C	-1.82714347	0.75196722	0.12572088
C	-0.63829200	1.53519068	-0.43291982
H	-1.89360396	-0.93619182	-1.20203664
H	1.89360396	0.93619182	-1.20203664
H	1.89360396	-0.93619182	1.20203664
H	-1.89360396	0.93619182	1.20203664
H	0.95980652	2.56980121	0.55829048
H	0.95980652	-2.56980121	-0.55829048
H	-0.95980652	-2.56980121	0.55829048
H	-0.95980652	2.56980121	-0.55829048
H	0.40469940	1.17558960	1.43845659
H	0.40469940	-1.17558960	-1.43845659
H	-0.40469940	-1.17558960	1.43845659
H	-0.40469940	1.17558960	-1.43845659
H	2.74449490	1.15712863	0.30715980
H	2.74449490	-1.15712863	-0.30715980
H	-2.74449490	-1.15712863	0.30715980
H	-2.74449490	1.15712863	-0.30715980



### 3.10 C<sub>8</sub>H<sub>16</sub>: Twist boat-chair / TBC / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	0.71975	45.00000	39.86465
3.	0.83337	22.50000	104.78115
4.	-0.21989		
Planar coordinates			
	t	tau	gamma
1.	0.06503	22.50000	22.68811
2.	0.06692	45.00000	25.48121
3.	0.09386	67.50000	41.94425
4.	0.01913	90.00000	10.55338
5.	0.04385	292.50000	25.27839
6.	0.09285	315.00000	0.00000
R	1.76717		

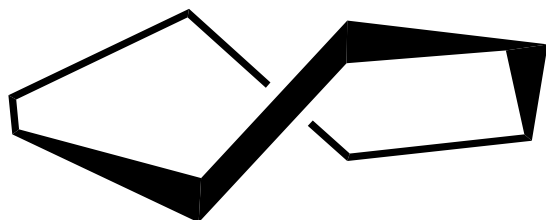
C	-0.76776590	-0.00628701	-1.45625752
C	0.76776590	0.00628701	-1.45625752
C	1.36413912	1.23238207	-0.76654149
C	0.76776590	1.56508305	0.60324055
C	0.65432702	0.40559414	1.60091171
C	-0.65432702	-0.40559414	1.60091171
C	-0.76776590	-1.56508305	0.60324055
C	-1.36413912	-1.23238207	-0.76654149
H	-0.75647764	-0.83146103	2.60061283
H	-1.50133940	0.27703252	1.48113763
H	1.50133940	-0.27703252	1.48113763
H	0.75647764	0.83146103	2.60061283
H	1.39326272	2.34320574	1.04490655
H	-0.21855795	2.01919651	0.48704447
H	0.21855795	-2.01919651	0.48704447
H	-1.39326272	-2.34320574	1.04490655
H	-2.44070323	-1.08279962	-0.65422944
H	-1.24175815	-2.10586540	-1.41216836
H	2.44070323	1.08279962	-0.65422944
H	1.24175815	2.10586540	-1.41216836
H	-1.15098973	0.04345538	-2.47599761
H	-1.13970608	0.89007402	-0.95942558
H	1.15098973	-0.04345538	-2.47599761
H	1.13970608	-0.89007402	-0.95942558



3.11 C<sub>8</sub>H<sub>16</sub>: Wiberg's transition state 1 / WT1 / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.13831	45.00000	65.20329
3.	0.27430	292.50000	31.43895
4.	0.44869		
Planar coordinates			
	t	tau	gamma
1.	0.00187	292.50000	0.47522
2.	0.16267	45.00000	46.20283
3.	0.04427	337.50000	16.48675
4.	0.05052	90.00000	19.73947
5.	0.00375	22.50000	1.52610
6.	0.14073	315.00000	0.00000
R	1.74846		

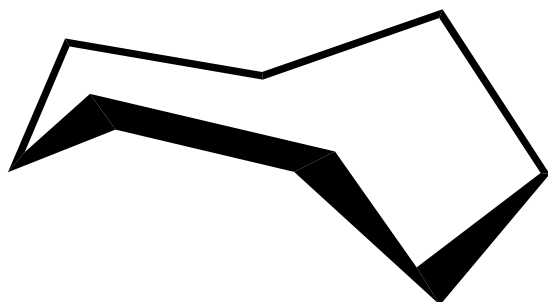
C	1.27548345	0.83268773	-0.52540247
C	1.55364623	-0.25874024	0.52659642
C	0.72991127	-0.25492486	1.82490767
C	-0.72991127	0.25492486	1.82490767
C	-1.55364623	0.25874024	0.52659642
C	-1.27548345	-0.83268773	-0.52540247
C	-0.72991127	-0.23932323	-1.82903118
C	0.72991127	0.23932323	-1.82903118
H	-2.20927694	-1.34358212	-0.76306093
H	2.20927694	1.34358212	-0.76306093
H	-2.60392722	0.21325839	0.81804164
H	2.60392722	-0.21325839	0.81804164
H	0.61063091	1.60071495	-0.13051203
H	-0.61063091	-1.60071495	-0.13051203
H	0.84610601	0.96285746	-2.63852011
H	-0.84610601	-0.96285746	-2.63852011
H	-1.26394750	-0.33490960	2.57129321
H	1.26394750	0.33490960	2.57129321
H	1.37925449	-0.60179733	-2.08542771
H	-1.37925449	0.60179733	-2.08542771
H	-0.74207668	1.27654109	2.20815456
H	0.74207668	-1.27654109	2.20815456
H	-1.44038301	1.22587883	0.03760870
H	1.44038301	-1.22587883	0.03760870



3.12 C<sub>8</sub>H<sub>16</sub>: Wiberg's transition state 2 / WT2 / C<sub>1</sub>

Puckering coordinates			
	q	phi	theta
2.	0.90687	66.27312	49.66313
3.	0.71883	27.96987	111.02144
4.	-0.27624		
Planar coordinates			
	t	tau	gamma
1.	0.05920	62.57080	24.46082
2.	0.01314	339.04034	5.79406
3.	0.10837	92.80806	56.82518
4.	0.05144	142.70676	46.55326
5.	0.04005	271.14549	55.28046
6.	0.02775	6.99474	0.00000
R	1.76120		

C	-0.27322488	1.73122373	-0.37060958
C	-1.15035496	1.04839512	0.68610663
C	-1.93614937	-0.13252001	0.12095916
C	-1.09218790	-1.15680682	-0.63018691
C	0.02756103	-1.79137003	0.20421116
C	1.42878895	-1.23728259	-0.05281894
C	1.73664244	0.17563530	0.44403287
C	1.23129170	1.35779897	-0.38998980
H	0.06062379	-2.86136458	-0.00733547
H	-0.20751597	-1.70422267	1.26921778
H	1.63588508	-1.28988314	-1.12637774
H	2.14251538	-1.91187754	0.42581059
H	2.82459845	0.27304966	0.46680530
H	1.41808515	0.27327247	1.48437020
H	1.54679067	1.19524463	-1.42326458
H	1.79153063	2.23015063	-0.04942998
H	-0.71143634	1.53587376	-1.35111170
H	-0.33769190	2.81084944	-0.23726631
H	-1.86383893	1.76851510	1.08895465
H	-0.54643418	0.72593554	1.53407828
H	-2.69977793	0.25633425	-0.55795960
H	-2.46825350	-0.63832906	0.93074308
H	-0.65807961	-0.69667626	-1.52171008
H	-1.76120297	-1.93731416	-0.99575200

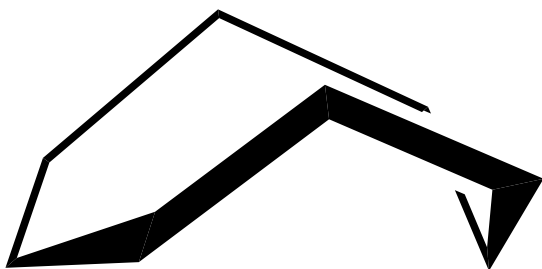




3.13  $C_8H_{16}$ : Wiberg's transition state 4 / WT4 /  $C_s$

Puckering coordinates			
	q	phi	theta
2.	1.41968	0.00000	78.83405
3.	0.24347	0.00000	119.67672
4.	-0.13874		
Planar coordinates			
	t	tau	gamma
1.	0.08016	0.00000	25.90440
2.	0.03692	180.00000	12.92523
3.	0.07592	0.00000	28.16207
4.	0.13932	0.00000	79.22288
5.	0.02611	0.00000	79.91977
6.	0.00464	0.00000	0.00000
R	1.70945		

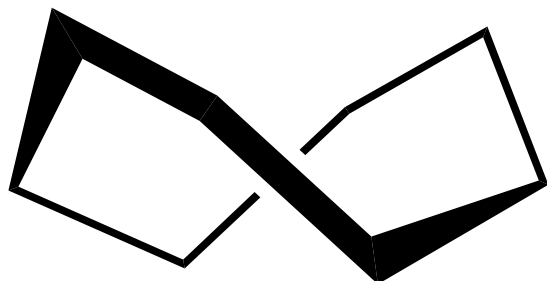
C	-1.46621601	0.69707384	0.00000000
C	-0.76385341	1.12458178	1.28261655
C	0.59761843	0.47723509	1.53786047
C	0.59761843	-1.04522507	1.39071139
C	0.61281082	-1.75401035	-0.00000000
C	0.59761843	-1.04522507	-1.39071139
C	0.59761843	0.47723509	-1.53786047
C	-0.76385341	1.12458178	-1.28261655
H	1.37617062	0.92946656	-0.92985658
H	1.37617062	0.92946656	0.92985658
H	-0.65906633	2.21306753	-1.28817951
H	-0.65906633	2.21306753	1.28817951
H	-1.41278252	0.87370679	-2.12604446
H	-1.41278252	0.87370679	2.12604446
H	-0.27075106	-1.41147397	-1.94460463
H	-0.27075106	-1.41147397	1.94460463
H	0.87422791	0.69613414	-2.57194011
H	0.87422791	0.69613414	2.57194011
H	1.46296102	-1.41700184	-1.94041145
H	1.46296102	-1.41700184	1.94041145
H	1.49931665	-2.38715220	-0.00000000
H	-0.22236839	-2.45445076	-0.00000000
H	-1.60295019	-0.38734606	0.00000000
H	-2.47168756	1.12366795	0.00000000



3.14 C<sub>8</sub>H<sub>16</sub>: S / S / S<sub>4</sub>

Puckering coordinates			
	q	phi	theta
2.	1.59501	18.45248	90.00000
3.	0.00000	0.00000	90.00000
4.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.17227	29.13178	90.00000
5.	0.00000	0.00000	0.00000
6.	0.00000	0.00000	0.00000
R	1.66034		

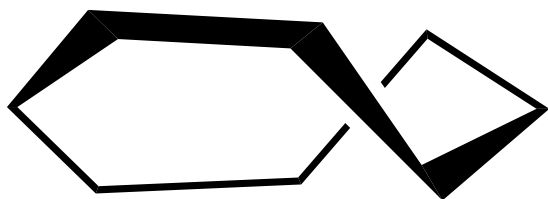
C	-1.06927808	1.06927808	0.75650449
C	-0.18415932	1.80337569	-0.25242540
C	1.06927808	1.06927808	-0.75650449
C	1.80337569	0.18415932	0.25242540
C	1.06927808	-1.06927808	0.75650449
C	0.18415932	-1.80337569	-0.25242540
C	-1.06927808	-1.06927808	-0.75650449
C	-1.80337569	-0.18415932	0.25242540
H	-1.82592817	1.77484138	1.10724553
H	-0.46795100	0.83820966	1.63336865
H	1.82592817	-1.77484138	1.10724553
H	0.46795100	-0.83820966	1.63336865
H	0.83820966	0.46795100	-1.63336865
H	1.77484138	1.82592817	-1.10724553
H	-0.83820966	-0.46795100	-1.63336865
H	-1.77484138	-1.82592817	-1.10724553
H	-0.78486518	2.10870503	-1.11378813
H	0.13952691	2.72929800	0.22891110
H	0.78486518	-2.10870503	-1.11378813
H	-0.13952691	-2.72929800	0.22891110
H	2.72929800	-0.13952691	-0.22891110
H	2.10870503	0.78486518	1.11378813
H	-2.72929800	0.13952691	-0.22891110
H	-2.10870503	-0.78486518	1.11378813



3.15 C<sub>8</sub>H<sub>16</sub>: New transition state 1 in this work / NT1 / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.13361	0.00000	66.21205
3.	0.49970	315.00000	90.00000
4.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.13794	45.00000	42.56411
2.	0.04382	270.00000	16.96101
3.	0.10217	315.00000	45.33033
4.	0.08648	0.00000	58.89763
5.	0.04075	45.00000	51.35653
6.	0.03258	90.00000	0.00000
R	1.76834		

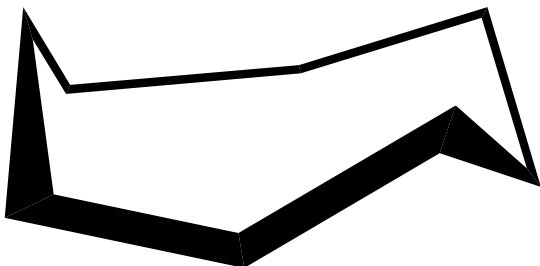
C	0.00000000	1.26099120	1.08959487
C	-0.00000000	-0.00000000	1.94665756
C	-0.00000000	-1.26099120	1.08959487
C	-1.25034856	-1.28912154	0.20982648
C	-1.12632819	-0.88128509	-1.27301858
C	0.00000000	0.00000000	-1.91577713
C	1.12632819	0.88128509	-1.27301858
C	1.25034856	1.28912154	0.20982648
H	-1.67706960	-2.29253357	0.21740605
H	-1.99970158	-0.65593906	0.68870712
H	1.99970158	0.65593906	0.68870712
H	1.67706960	2.29253357	0.21740605
H	1.10399245	1.80565722	-1.85020443
H	2.07676240	0.41597967	-1.53572333
H	-2.07676240	-0.41597967	-1.53572333
H	-1.10399245	-1.80565722	-1.85020443
H	0.90379167	-1.31062636	0.47828593
H	0.02091819	-2.13635760	1.73959629
H	-0.02091819	2.13635760	1.73959629
H	-0.90379167	1.31062636	0.47828593
H	-0.87833296	-0.02290433	2.59664442
H	0.87833296	0.02290433	2.59664442
H	-0.54158640	0.66633821	-2.58576991
H	0.54158640	-0.66633821	-2.58576991



3.16 C<sub>8</sub>H<sub>16</sub>: New transition state 2 in this work / NT2 / C<sub>s</sub>

Puckering coordinates			
	q	phi	theta
2.	0.38464	0.00000	23.26277
3.	0.87643	0.00000	101.60228
4.	-0.17994		
Planar coordinates			
	t	tau	gamma
1.	0.01462	0.00000	5.13518
2.	0.10090	0.00000	38.34454
3.	0.05753	0.00000	26.80971
4.	0.01291	0.00000	6.50935
5.	0.01167	0.00000	5.92153
6.	0.11251	0.00000	0.00000
R	1.81236		

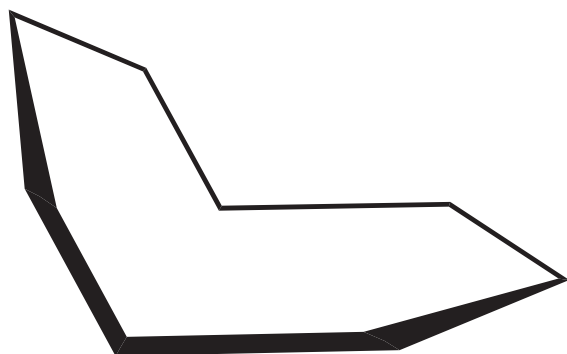
C	1.20304065	-1.06253974	0.00000000
C	0.40807147	-1.29830281	1.29591869
C	-0.24007934	-0.08989284	2.01285801
C	-0.24007934	1.25955975	1.30181163
C	-1.05177204	1.33456752	-0.00000000
C	-0.24007934	1.25955975	-1.30181163
C	-0.24007934	-0.08989284	-2.01285801
C	0.40807147	-1.29830281	-1.29591869
H	2.02992624	-1.77353898	0.00000000
H	1.66981252	-0.07724083	0.00000000
H	-1.81843974	0.55400048	-0.00000000
H	-1.59371849	2.28068718	-0.00000000
H	-1.27558009	-0.33539795	2.25709272
H	0.26109389	0.05100227	2.97202154
H	-1.27558009	-0.33539795	-2.25709272
H	0.26109389	0.05100227	-2.97202154
H	-0.35832223	-2.04321932	1.07589106
H	1.07358854	-1.77768883	2.01423374
H	-0.64982794	1.98089915	2.01128143
H	0.78397491	1.58818280	1.11065995
H	-0.64982794	1.98089915	-2.01128143
H	0.78397491	1.58818280	-1.11065995
H	-0.35832223	-2.04321932	-1.07589106
H	1.07358854	-1.77768883	-2.01423374



3.17  $C_8H_{16}$ : New transition state 3 in this work / NT3 /  $C_{2v}$

Puckering coordinates			
	q	phi	theta
2.	1.14302	0.00000	74.18774
3.	0.00000	0.00000	0.00000
4.	0.32371		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.12817	0.00000	50.12684
3.	0.00000	0.00000	0.00000
4.	0.07991	0.00000	48.27979
5.	0.00000	0.00000	0.00000
6.	0.07125	0.00000	0.00000
R	1.80850		

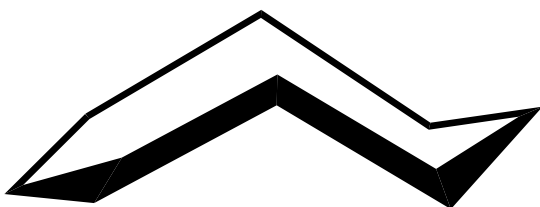
C	0.00000000	1.52917673	0.69090945
C	1.29506254	1.37555541	-0.10949532
C	1.92800456	-0.00000000	-0.45211033
C	1.29506254	-1.37555541	-0.10949532
C	-0.00000000	-1.52917673	0.69090945
C	-1.29506254	-1.37555541	-0.10949532
C	-1.92800456	0.00000000	-0.45211033
C	-1.29506254	1.37555541	-0.10949532
H	-2.12960509	0.00000000	-1.52290004
H	-2.91399440	0.00000000	0.01025880
H	2.12960509	-0.00000000	-1.52290004
H	2.91399440	-0.00000000	0.01025880
H	0.00000000	2.56737500	1.03273285
H	0.00000000	0.93305659	1.59923150
H	-0.00000000	-2.56737500	1.03273285
H	-0.00000000	-0.93305659	1.59923150
H	-1.13638537	1.92236239	-1.04195942
H	-2.05982168	1.94257645	0.42287243
H	1.13638537	1.92236239	-1.04195942
H	2.05982168	1.94257645	0.42287243
H	1.13638537	-1.92236239	-1.04195942
H	2.05982168	-1.94257645	0.42287243
H	-1.13638537	-1.92236239	-1.04195942
H	-2.05982168	-1.94257645	0.42287243



3.18 C<sub>8</sub>H<sub>16</sub>: New transition state 4 in this work / NT4 / C<sub>s</sub>

Puckering coordinates			
	q	phi	theta
2.	0.76721	180.00000	49.45373
3.	0.33831	0.00000	31.02848
4.	0.56242		
Planar coordinates			
	t	tau	gamma
1.	0.03190	0.00000	11.13092
2.	0.12275	180.00000	49.21510
3.	0.03381	180.00000	18.61703
4.	0.03770	0.00000	22.06358
5.	0.02213	180.00000	13.76556
6.	0.09034	180.00000	0.00000
R	1.81942		

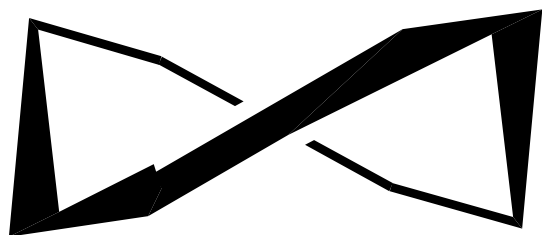
C	0.17421979	-2.01717660	0.00000000
C	-0.19771632	-1.28598906	1.28207179
C	0.58738293	0.00487278	1.56863315
C	-0.19771632	1.30559648	1.39012923
C	-0.53092414	1.92418024	-0.00000000
C	-0.19771632	1.30559648	-1.39012923
C	0.58738293	0.00487278	-1.56863315
C	-0.19771632	-1.28598906	-1.28207179
H	-1.60061831	2.13119426	-0.00000000
H	-0.06590292	2.90895824	-0.00000000
H	1.24949434	-2.21941011	0.00000000
H	-0.32084380	-2.99095882	0.00000000
H	1.52052438	0.02119375	1.00664289
H	0.88397956	-0.01074836	2.61894520
H	1.52052438	0.02119375	-1.00664289
H	0.88397956	-0.01074836	-2.61894520
H	0.33936250	2.07458773	1.94709083
H	-1.13605748	1.16749242	1.93151286
H	-0.05252416	-1.97599207	2.11494184
H	-1.26793816	-1.05931739	1.26341344
H	-0.05252416	-1.97599207	-2.11494184
H	-1.26793816	-1.05931739	-1.26341344
H	0.33936250	2.07458773	-1.94709083
H	-1.13605748	1.16749242	-1.93151286



3.19 C<sub>8</sub>H<sub>16</sub>: New transition state 5 in this work / NT5 / D<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.39631	45.00000	77.23306
3.	0.00000	0.00000	180.00000
4.	-0.31639		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.16557	225.00000	46.67270
3.	0.00000	0.00000	0.00000
4.	0.08559	90.00000	33.23296
5.	0.00000	0.00000	0.00000
6.	0.13063	135.00000	0.00000
R	1.70676		

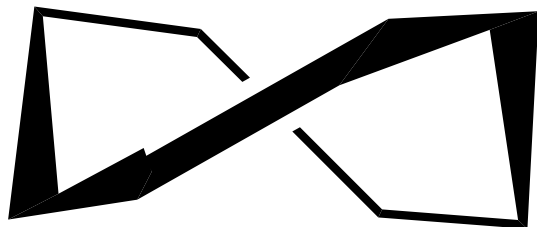
C	1.79364903	0.67705125	0.38181147
C	1.79364903	-0.67705125	-0.38181147
C	0.47109724	-1.42554784	-0.60553115
C	-0.47109724	-1.42554784	0.60553115
C	-1.79364903	-0.67705125	0.38181147
C	-1.79364903	0.67705125	-0.38181147
C	-0.47109724	1.42554784	-0.60553115
C	0.47109724	1.42554784	0.60553115
H	2.46153509	1.34923233	-0.15956559
H	2.26083305	0.53243609	1.35720190
H	2.46153509	-1.34923233	0.15956559
H	2.26083305	-0.53243609	-1.35720190
H	-2.46153509	-1.34923233	-0.15956559
H	-2.26083305	-0.53243609	1.35720190
H	-2.46153509	1.34923233	0.15956559
H	-2.26083305	0.53243609	-1.35720190
H	0.72685622	-2.45059414	-0.87752089
H	-0.05460054	-1.02182000	-1.46977380
H	-0.05460054	1.02182000	1.46977380
H	0.72685622	2.45059414	0.87752089
H	-0.72685622	-2.45059414	0.87752089
H	0.05460054	-1.02182000	1.46977380
H	0.05460054	1.02182000	-1.46977380
H	-0.72685622	2.45059414	-0.87752089



3.20 C<sub>8</sub>H<sub>16</sub>: New transition state 6 in this work / NT6 / C<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	1.51918	45.00000	80.91612
3.	0.12529	22.50000	148.94919
4.	-0.20809		
Planar coordinates			
	t	tau	gamma
1.	0.01875	22.50000	5.17592
2.	0.12635	225.00000	37.61494
3.	0.04068	67.50000	14.36209
4.	0.11355	90.00000	45.62843
5.	0.00723	292.50000	3.73046
6.	0.11085	135.00000	0.00000
R	1.68021		

C	-1.81016599	0.14166162	0.52327046
C	-1.38015049	1.17981087	-0.52327040
C	0.12069701	1.54716197	-0.59157876
C	0.95427283	1.13582841	0.62999762
C	1.88555530	-0.06388854	0.40348582
C	1.37846495	-1.28811285	-0.40348588
C	-0.12837920	-1.47792466	-0.62999763
C	-1.00866302	-1.17935430	0.59157878
H	-2.85653449	-0.08900490	0.31557878
H	-1.80997551	0.60718098	1.50974509
H	-1.95693887	2.08281101	-0.31557869
H	-1.70918775	0.85050431	-1.50974502
H	2.77999590	0.30408337	-0.10241628
H	2.22782330	-0.40209266	1.38284543
H	1.75073453	-2.18077331	0.10241620
H	1.85963137	-1.29098645	-1.38284551
H	0.19611614	2.62508224	-0.73387219
H	0.56816077	1.10477241	-1.48265704
H	-0.37944166	-1.18294233	1.48265704
H	-1.71753838	-1.99488840	0.73387222
H	1.58479114	1.97034107	0.93999621
H	0.29610772	0.94526029	1.47575980
H	-0.45902022	-0.87777962	-1.47575979
H	-0.27262502	-2.51385799	-0.93999624

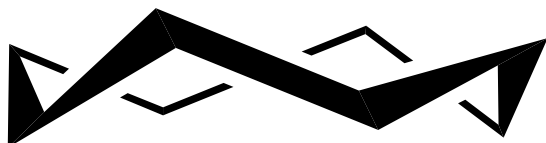




3.21 C<sub>8</sub>H<sub>16</sub>: New transition state 7 in this work / NT7 / D<sub>2</sub>

Puckering coordinates			
	q	phi	theta
2.	0.20245	45.00000	14.09379
3.	0.00000	0.00000	0.00000
4.	0.80637		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.04937	45.00000	44.36576
3.	0.00000	0.00000	0.00000
4.	0.00029	90.00000	0.33072
5.	0.00000	0.00000	0.00000
6.	0.05047	315.00000	0.00000
R	1.84517		

C	-0.67955219	1.63930469	0.35667374
C	0.67955219	1.63930469	-0.35667374
C	1.77035488	0.73214435	0.21351738
C	1.77035488	-0.73214435	-0.21351738
C	0.67955219	-1.63930469	0.35667374
C	-0.67955219	-1.63930469	-0.35667374
C	-1.77035488	-0.73214435	0.21351738
C	-1.77035488	0.73214435	-0.21351738
H	-1.06615871	2.65904099	0.31693455
H	-0.53664366	1.41779375	1.41861127
H	1.06615871	2.65904099	-0.31693455
H	0.53664366	1.41779375	-1.41861127
H	1.06615871	-2.65904099	0.31693455
H	0.53664366	-1.41779375	1.41861127
H	-1.06615871	-2.65904099	-0.31693455
H	-0.53664366	-1.41779375	-1.41861127
H	1.74671992	0.78867091	1.30615615
H	2.73398872	1.14968647	-0.08677734
H	-2.73398872	1.14968647	0.08677734
H	-1.74671992	0.78867091	-1.30615615
H	1.74671992	-0.78867091	-1.30615615
H	2.73398872	-1.14968647	0.08677734
H	-2.73398872	-1.14968647	-0.08677734
H	-1.74671992	-0.78867091	1.30615615



3.22 C<sub>8</sub>H<sub>16</sub>: Plane / P / D<sub>8h</sub>

```

      Puckering coordinates
            q            phi            theta
2.      0.00000      0.00000      90.00000
3.      0.00000      0.00000      90.00000
4.      0.00000
      Planar coordinates
            t            tau            gamma
1.      0.00000      0.00000      0.00000
2.      0.00000      0.00000      0.00000
3.      0.00000      0.00000      0.00000
4.      0.00000      0.00000      0.00000
5.      0.00000      0.00000      0.00000
6.      0.00000      0.00000
R      2.03967

```

C	-0.00000000	2.03967199	0.00000000
C	-1.44226590	1.44226590	0.00000000
C	-2.03967199	0.00000000	0.00000000
C	-1.44226590	-1.44226590	0.00000000
C	-0.00000000	-2.03967199	0.00000000
C	1.44226590	-1.44226590	0.00000000
C	2.03967199	-0.00000000	0.00000000
C	1.44226590	1.44226590	0.00000000
H	0.00000000	2.71073887	0.85704892
H	0.00000000	2.71073887	-0.85704892
H	-1.91678184	1.91678184	0.85704892
H	-1.91678184	1.91678184	-0.85704892
H	-2.71073887	0.00000000	0.85704892
H	-2.71073887	0.00000000	-0.85704892
H	-1.91678184	-1.91678184	0.85704892
H	-1.91678184	-1.91678184	-0.85704892
H	-0.00000000	-2.71073887	0.85704892
H	-0.00000000	-2.71073887	-0.85704892
H	1.91678184	-1.91678184	0.85704892
H	1.91678184	-1.91678184	-0.85704892
H	2.71073887	-0.00000000	0.85704892
H	2.71073887	-0.00000000	-0.85704892
H	1.91678184	1.91678184	0.85704892
H	1.91678184	1.91678184	-0.85704892

## 4 Cyclo[18]carbon ( $C_{18}$ )

### 4.1 $C_{18}$ : Cumulene / C / $D_{18h}$

Puckering coordinates			
	q	phi	theta
2.	0.00000	0.00000	90.00000
3.	0.00000	0.00000	90.00000
4.	0.00000	0.00000	90.00000
5.	0.00000	0.00000	90.00000
6.	0.00000	0.00000	90.00000
7.	0.00000	0.00000	90.00000
8.	0.00000	0.00000	90.00000
9.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.00000	0.00000	0.00000
5.	0.00000	0.00000	0.00000
6.	0.00000	0.00000	0.00000
7.	0.00000	0.00000	0.00000
8.	0.00000	0.00000	0.00000
9.	0.00000	0.00000	0.00000
10.	0.00000	0.00000	0.00000
11.	0.00000	0.00000	0.00000
12.	0.00000	0.00000	0.00000
13.	0.00000	0.00000	0.00000
14.	0.00000	0.00000	0.00000
15.	0.00000	0.00000	0.00000
16.	0.00000	0.00000	0.00000
R	3.67340		

C	-3.673400	0.000000	0.000000
C	-3.451867	1.256377	0.000000
C	-2.813988	2.361216	0.000000
C	-1.836700	3.181258	0.000000
C	-0.637879	3.617593	0.000000
C	0.637879	3.617593	0.000000
C	1.836700	3.181258	0.000000
C	2.813988	2.361216	0.000000
C	3.451867	1.256377	0.000000
C	3.673400	0.000000	0.000000
C	3.451867	-1.256377	0.000000
C	2.813988	-2.361216	0.000000
C	1.836700	-3.181258	0.000000
C	0.637879	-3.617593	0.000000
C	-0.637879	-3.617593	0.000000
C	-1.836700	-3.181258	0.000000
C	-2.813988	-2.361216	0.000000
C	-3.451867	-1.256377	0.000000

## 4.2 C<sub>18</sub>: Polyne / P / D<sub>9h</sub>

Puckering coordinates			
	q	phi	theta
2.	0.00000	0.00000	90.00000
3.	0.00000	0.00000	90.00000
4.	0.00000	0.00000	90.00000
5.	0.00000	0.00000	90.00000
6.	0.00000	0.00000	90.00000
7.	0.00000	0.00000	90.00000
8.	0.00000	0.00000	90.00000
9.	0.00000		
Planar coordinates			
	t	tau	gamma
1.	0.00000	0.00000	0.00000
2.	0.00000	0.00000	0.00000
3.	0.00000	0.00000	0.00000
4.	0.00000	0.00000	0.00000
5.	0.00000	0.00000	0.00000
6.	0.00000	0.00000	0.00000
7.	0.00000	0.00000	0.00000
8.	0.00000	0.00000	0.00000
9.	0.03083	90.00000	89.99949
10.	0.00000	0.00000	0.00000
11.	0.00000	0.00000	0.00000
12.	0.00000	0.00000	0.00000
13.	0.00000	0.00000	0.00000
14.	0.00000	0.00000	0.00000
15.	0.00000	0.00000	0.00000
16.	0.00000	0.00000	0.00000
R	3.69704		

C	-3.697042	0.030832	0.000000
C	-3.484628	1.235490	0.000000
C	-2.812280	2.400031	0.000000
C	-1.875222	3.186316	0.000000
C	-0.611621	3.646229	0.000000
C	0.611621	3.646229	0.000000
C	1.875222	3.186316	0.000000
C	2.812280	2.400031	0.000000
C	3.484628	1.235490	0.000000
C	3.697042	0.030832	0.000000
C	3.463538	-1.293435	0.000000
C	2.851917	-2.352794	0.000000
C	1.821820	-3.217148	0.000000
C	0.672348	-3.635521	0.000000
C	-0.672348	-3.635521	0.000000
C	-1.821820	-3.217148	0.000000
C	-2.851917	-2.352794	0.000000
C	-3.463538	-1.293435	0.000000