

Cycloalkanes C_nH_{2n} -----> $nCO_2 + nH_2O$ (kcal/mol)

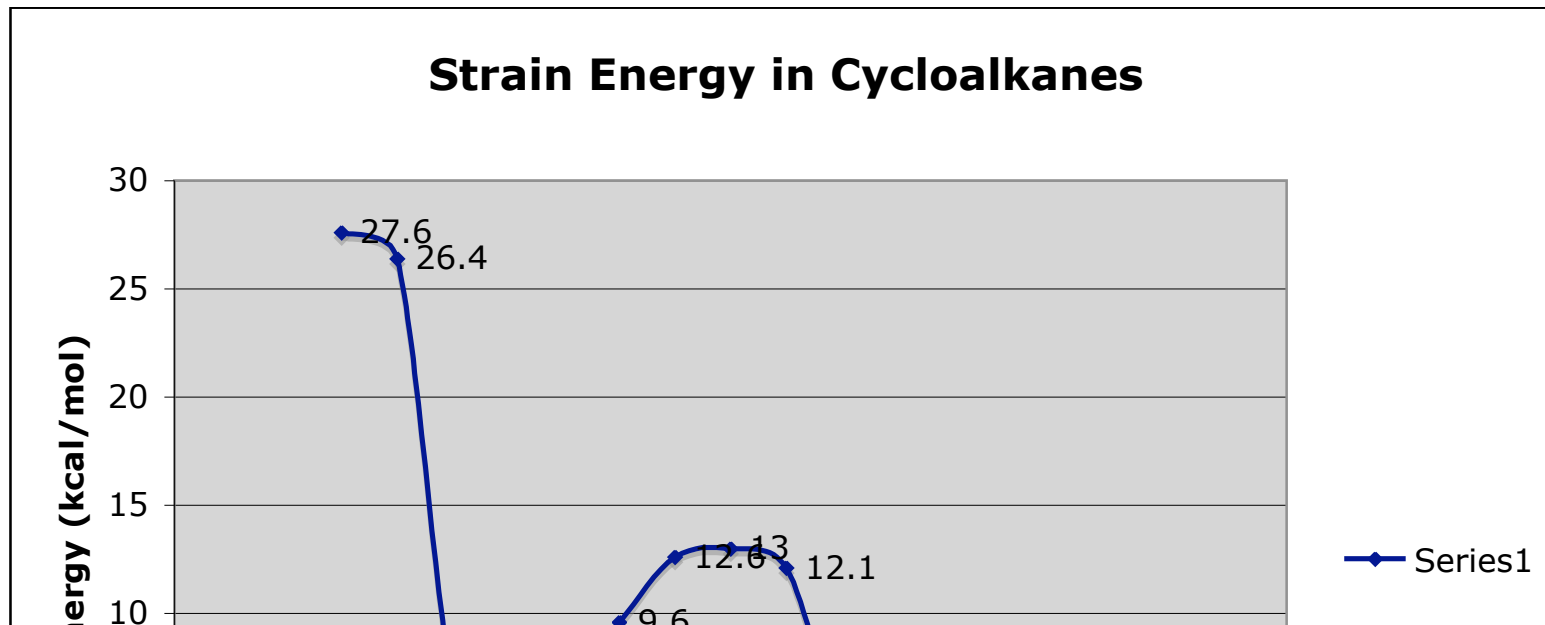
Ring Size	C + H ₂ + O ₂ from Std. State	ΔH_f°	ΔH_{comb}°	$ \Delta H_{comb}^\circ/CH_2 $	Strain/CH ₂	Total Strain	$\Delta H_f^\circ CO_2$ -94.05 $\Delta H_f^\circ H_2O$ -68.3
3	-487.05	12.7	-499.8	166.6	9.2	27.6	
4	-649.4	6.6	-656	164	6.6	26.4	
5	-811.75	-18.3	-793.5	158.7	1.3	6.5	
6	-974.1	-29.5	-944.6	157.4	0	0	
7	-1136.45	-28.2	-1108.3	158.3	0.9	6.3	
8	-1298.8	-29.7	-1269.1	158.6	1.2	9.6	
9	-1461.15	-31.8	-1429.4	158.8	1.4	12.6	
10	-1623.5	-36.9	-1586.6	158.7	1.3	13	
11	-1785.85	-42.9	-1743	158.5	1.1	12.1	
12	-1948.2	-55.1	-1893.1	157.8	0.4	4.8	
13	-2110.55	-58.9	-2051.7	157.8	0.4	5.2	
14	-2272.9	-65.6	-2207.3	157.7	0.3	4.2	
15	-2435.25	-72.1	-2363.2	157.5	0.1	1.5	
16	-2597.6	-77	-2520.6	157.5	0.1	1.6	
17	-2759.95	-87.2	-2672.8	157.2	-0.2	-3.4	

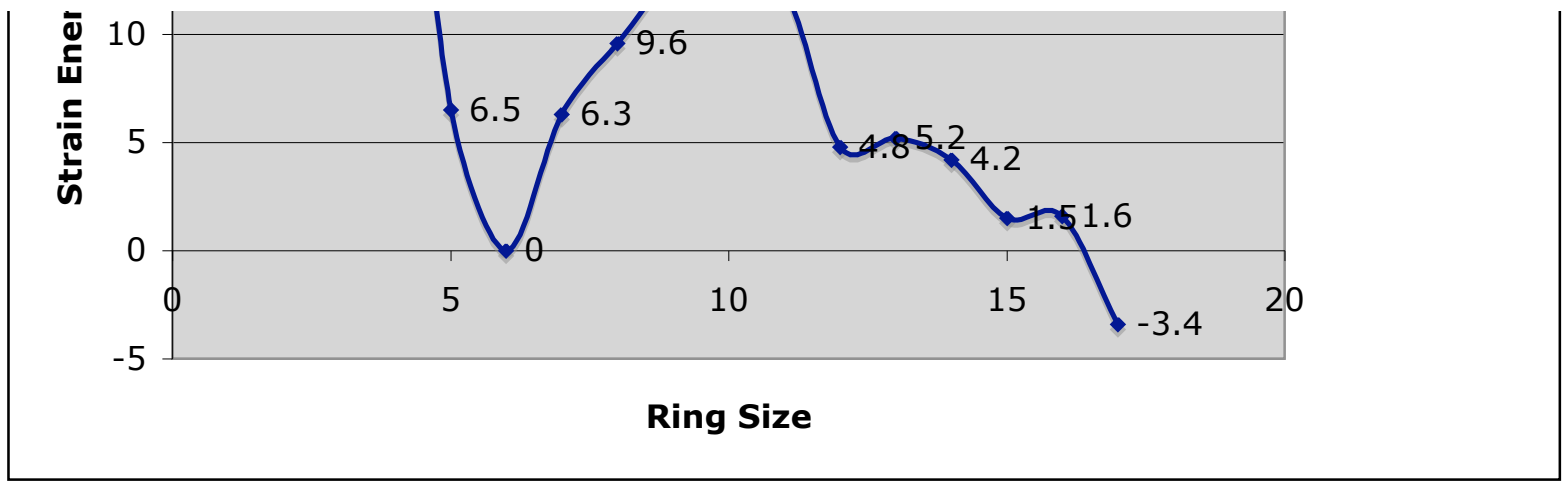
n-Alkanes C_nH_{2n+2} -----> $nCO_2 + (n+1)H_2O$

Chain Length	C + H ₂ + O ₂ from Std. State	ΔH_f°	ΔH_{comb}°	$\Delta(\Delta H_{comb}^\circ)/CH_2 $
2	-393	-20	-373	
3	-555.35	-25	-530.4	157.4

4	-717.7	-30	-687.7	157.3
5	-880.05	-35.1	-845	157.3
6	-1042.4	-40	-1002.4	157.4
7	-1204.75	-44.9	-1159.9	157.5
8	-1367.1	-49.9	-1317.2	157.3
9	-1529.45	-54.6	-1474.9	157.7
10	-1691.8	-59.7	-1632.1	157.2
11	-1854.15	-64.8	-1789.4	157.3
12	-2016.5	-69.2	-1947.3	157.9
16	-2665.9	-89.7	-2576.2	157.2
18	-2990.6	-99.2	-2891.4	157.6
32	-5263.5	-166.8	-5096.7	157.5

Average **157.4**





Ring Size Total Strain

3	27.6
4	26.4
5	6.5
6	0
7	6.3
8	9.6
9	12.6
10	13

11	12.1
12	4.8
13	5.2
14	12.6
15	1.5
16	1.6
17	3.4

3	27.6	-77	-2683	157.8	0.4	6.8
4	26.4	-78	-2682	157.8	0.4	6.8
5	6.5	-79	-2681	157.7	0.3	5.1
6	0	-80	-2680	157.6	0.2	3.4
7	6.3	-81	-2679	157.6	0.2	3.4
8	9.6	-82	-2678	157.5	0.1	1.7
9	12.6	-83	-2677	157.5	0.1	1.7
10	13	-84	-2676	157.4	0	0
11	12.1	-85	-2675	157.4	0	0
12	4.8	-86	-2674	157.3	-0.1	-1.7
13	5.2	-87	-2673	157.2	-0.2	-3.4
14	4.2	-88	-2672	157.2	-0.2	-3.4
15	1.5	-89	-2671	157.1	-0.3	-5.1
16	1.6	-90	-2670	157.1	-0.3	-5.1
17	-3.4	-91	-2669	157	-0.4	-6.8
		-92	-2668	156.9	-0.5	-8.5
		-93	-2667	156.9	-0.5	-8.5
		-94	-2666	156.8	-0.6	-10.2

