Conformations of cycloalkanes

- Baeyer observed that the planar arrays of $sp^3$-hybridized carbons which make up the constitutions of cycloalkanes are generally distorted from the tetrahedral geometry:

$$\angle CCC = \frac{180(n-2)}{n}^\circ,$$

where $n$ = the number of C in the cycloalkane parent ring.

- So, the relative thermodynamic stability of cycloalkanes ($\Delta E / CH_2$) should vary as a function of the Baeyer angle or ring strain.
Obviously, Baeyer’s predictions were not accurate! Why?

• Cycloalkanes are not necessarily flat: they may be able to make conformational changes that can reduce ring strain.

• The thermodynamic stability of a molecule is a function of

  \[ \text{angle strain} + \text{torsional strain} + \text{steric interactions} \]

• These factors are not independent: changing one can increase or decrease the others

• Molecules will adjust their conformations so as to minimize strains and interactions.

• Cyclohexane appears to be able to adopt a conformation with no angle strain. Can this conformation be determined?