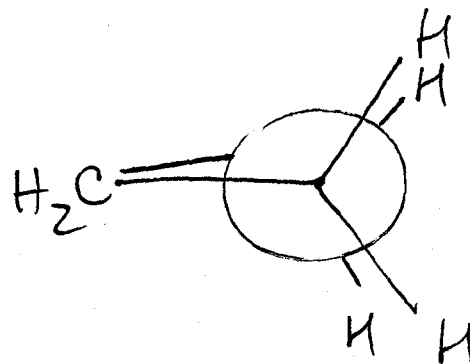
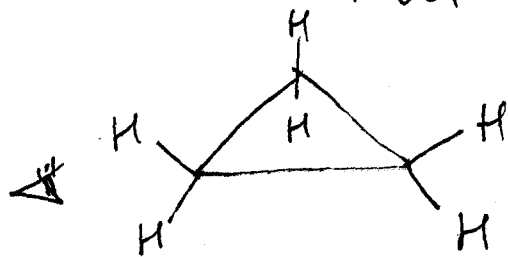


cyclopropane - flat.



all
eclipsed

very strained
molecule

What is "ring strain"?

Two components.

1. angle strain - caused by distortion of bond angles away from tetrahedral.

(cyclopropane: 60° vs 109.5°)

2. steric strain - caused by eclipsing hydrogens / substituents

How can we quantify this?

We can measure the heat of combustion for straight-chain alkanes. For every CH_2 added to the chain, ΔH° increases by about 157 kcal/mol.

propane: $\Delta H = -530.6$

butane: -687.4

pentane: -845.2

Since cyclic alkanes have formula $(\text{CH}_2)_n$ we should be able to predict ΔH for combustion

<u>Ring</u>	<u>Predicted</u>	<u>Observed</u>	<u>Δ</u>
cyclopropane	-472.2 kcal/mol	-499.8	27.6 kcal/mol
cyclobutane	-629.6	-655.9	26.3
cyclohexane	-944.4	-944.5	0.1
			\uparrow ring strain

Look @ lots of examples:

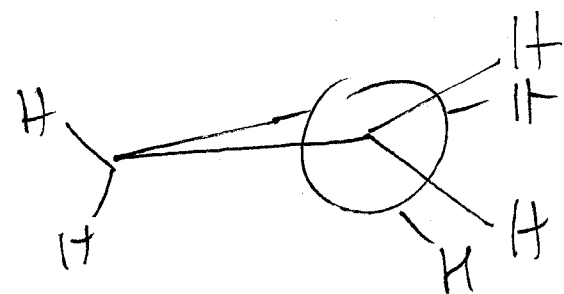
Small rings (3,4) - highly strained

Common rings (5,6,7) - little strain

Medium rings (8-12) - strained

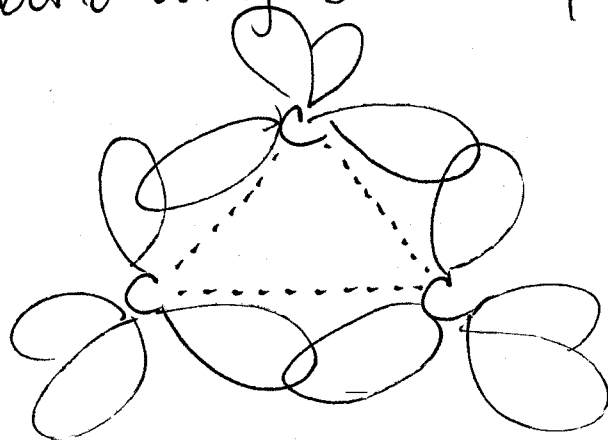
Large rings (>12) - little strain

cyclopropane



C-C bonds in cyclopropane are relatively weak (not formed by max. orbital overlap)

60° bond angles - very distorted.

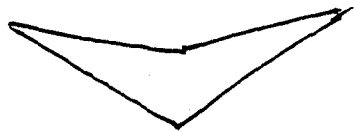


"banana bonds"

DH° (bond strength)
 $= 65 \text{ kcal/mol}$

Compare: 90 kcal/mol in ethane

cyclobutane - not planar - puckered

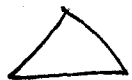


bent 26° out of planarity.

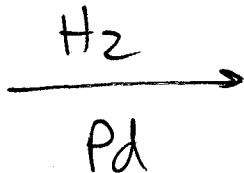
- decreases bond angles (thereby increases that component of ring strain)

$$\Delta H^\circ = 63 \text{ kcal/mol}$$

- lets H's get away from being eclipsed (decreases the steric/torsional strain)



or



cyclopentane



- might be expected to be planar
(108° bond angles) - but the
steric/torsional strain would
be very high.

Instead, it is also puckered.

This increases the angle
strain somewhat, but
greatly decreases the steric strain.



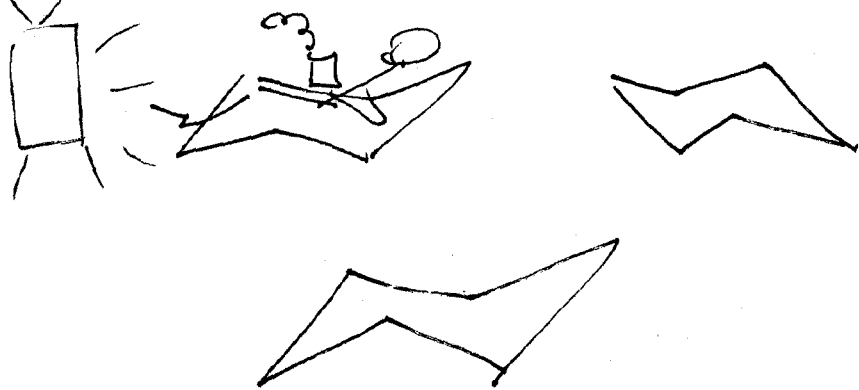
Overall - very little strain.

cyclohexane

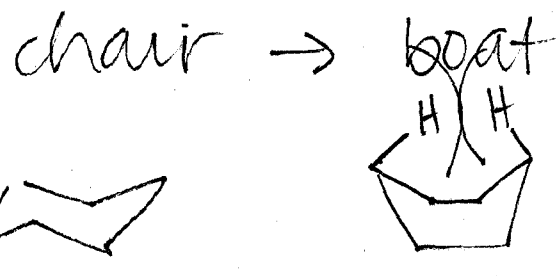


Strain-free

most stable conformation
called "chair" -
tetrahedral bond angles
zero eclipsing interactions.



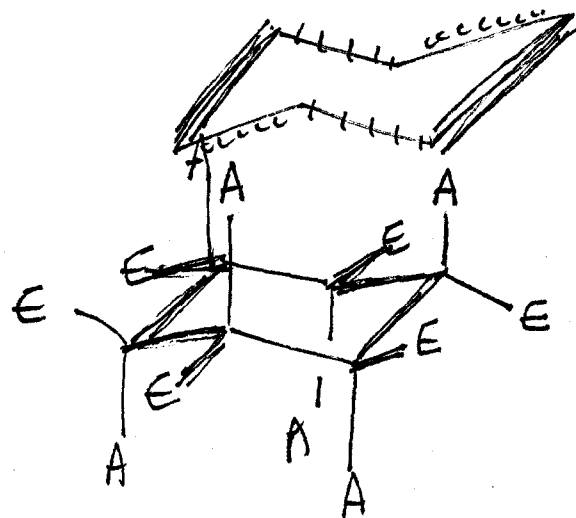
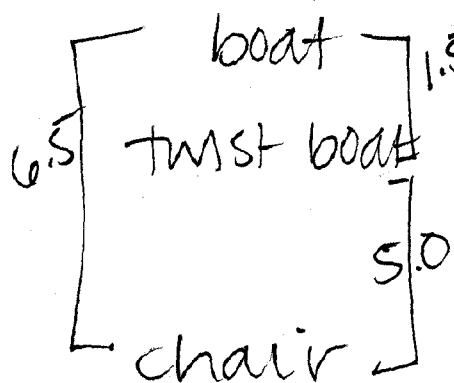
conformational change -



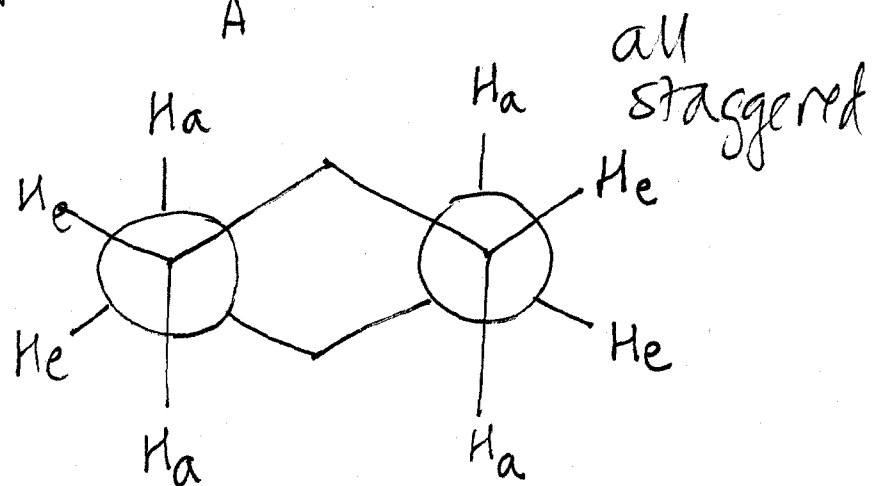
bowsprit

H's -
steric problems.

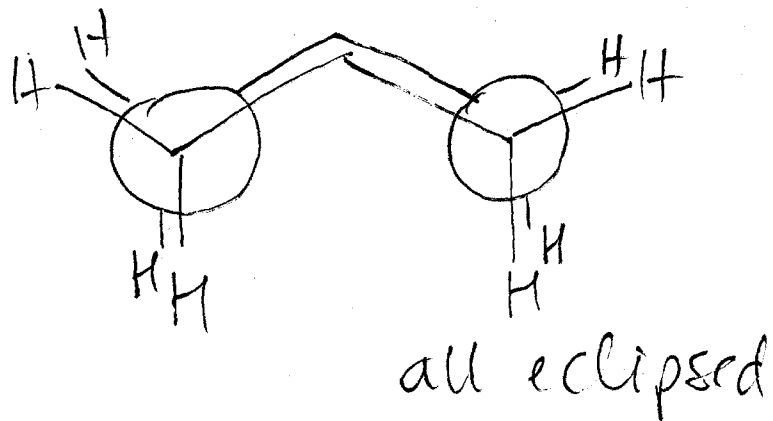
(transannular strain)



chair \rightarrow



boat \rightarrow



"ring flip" - convert one chair into the other
this interconverts axial + equat

