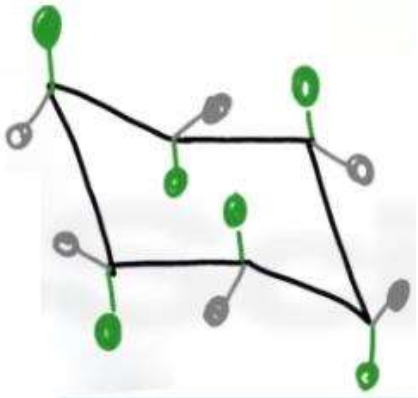
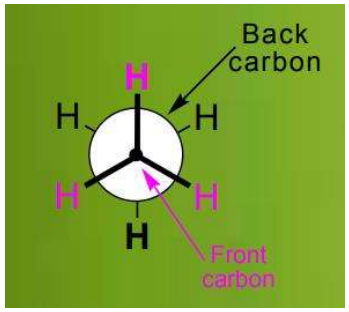


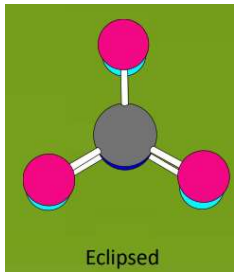
Conformational Analysis of Cyclohexane

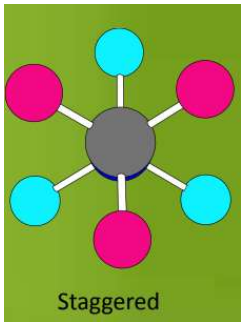
Upasana Borthakur

Structures that can be interconverted simply by rotation about single bonds at room temperature without involving a bond breaking process are called conformations of the same molecule.

Example-Conformations of ethane







***Stability**: staggered>eclipsed*

Reason

***Steric hindrance(Van der waals repulsion)-** In the eclipsed conformation, the positioning of the atoms forces them closer together, increasing the amount of steric strain in the molecule and strain caused by this effect is called torsional strain.*

***Bond pair-Bond pair repulsion(torsional repulsion)** -The electrons in the bonds repel each other and this is maximum in eclipsed form and strain caused by this effect is called torsional strain.*

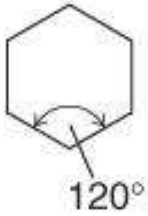
Cyclohexane (C_6H_{12})

Baeyer Strain Theory- *Baeyer proposed "any deviation of bond angle from ideal bond angle value (109.5˚) will produce a strain in molecule. The strain is also called as* ***angle strain****.*

❖ *The bond angel is of 109˚ 28' (or 109.5˚) for sp^3 carbon atom in tetrahedral geometry*

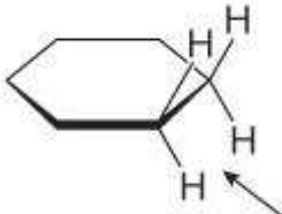
If a cyclohexane ring were flat....

angle strain



The internal bond angle is >109.5°.

torsional strain



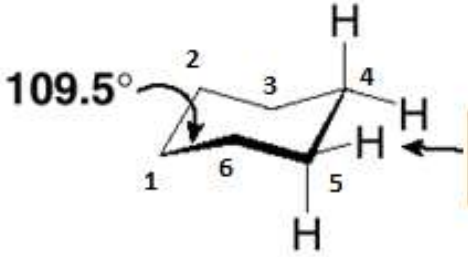
All H's are aligned.

3 *up* C's and 3 *down* C's

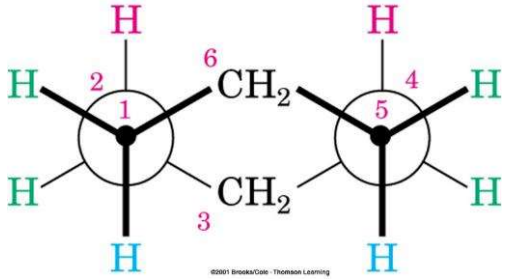
● = *up* C ○ = *down* C

In reality, cyclohexane adopts a puckered "chair" conformation, which is more stable than any possible other conformation.

The chair conformation is so stable because it eliminates angle strain (all C—C—C angles are 109.5°), and torsional strain (all hydrogens on adjacent C atoms are staggered).

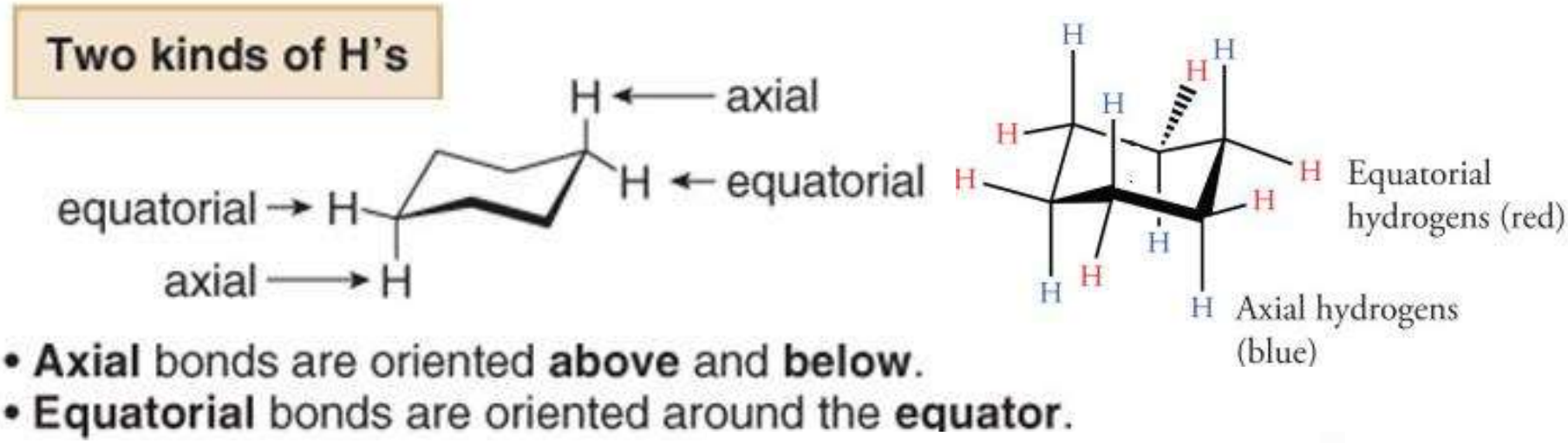


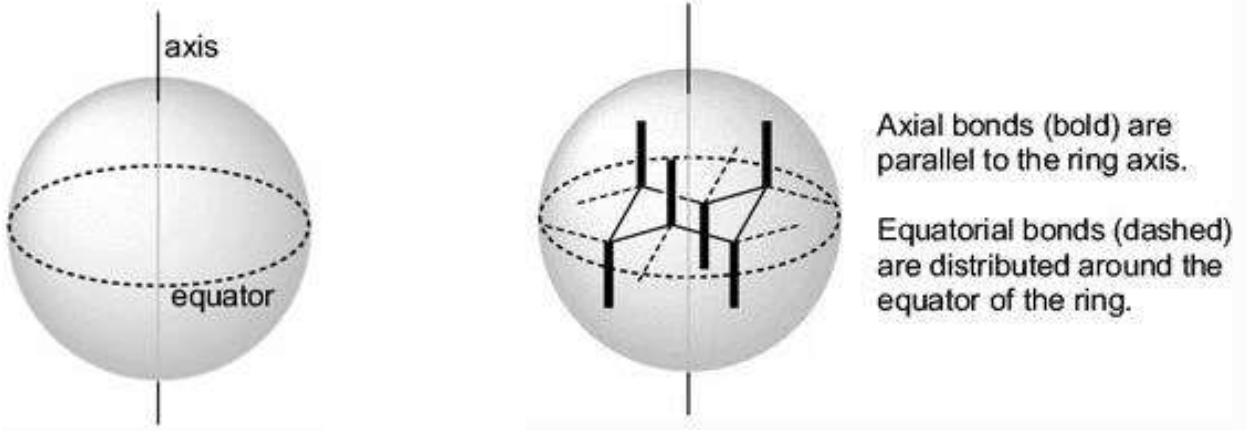
All H's are **staggered.**



In cyclohexane, each C has two different kinds of hydrogens: (1) axial hydrogens are located above and below the ring (along a perpendicular axis) i.e pointing up and down; (2) equatorial hydrogens are located in the plane of the ring and pointing sideways(around the equator).

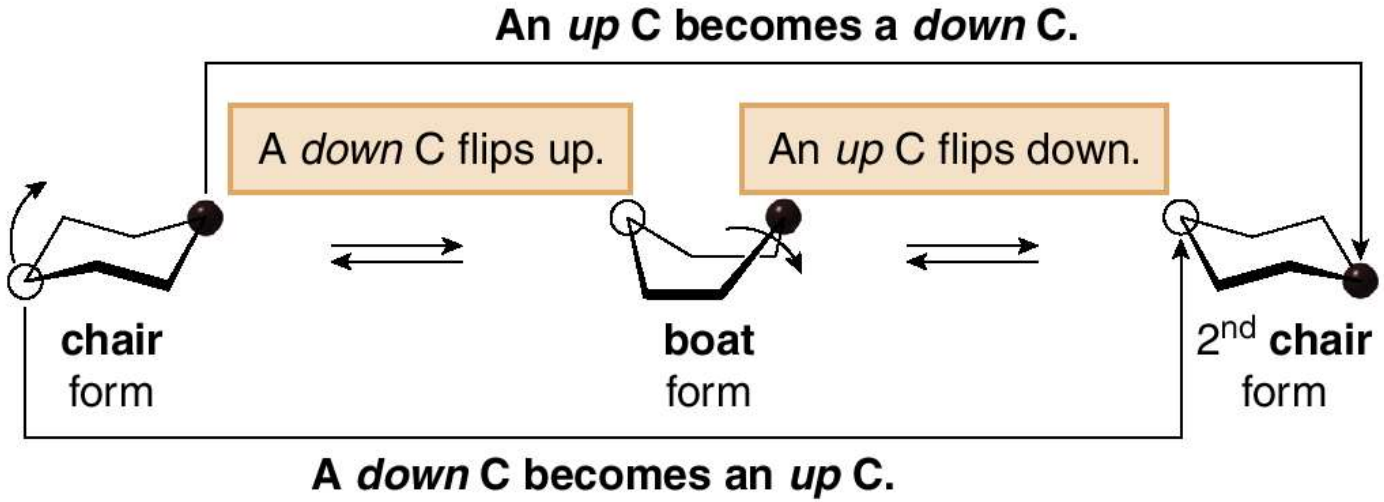
Each of the C's has one equatorial 'H' and one axial 'H'. If one is above the plane of molecule then other is below in an alternative passion.

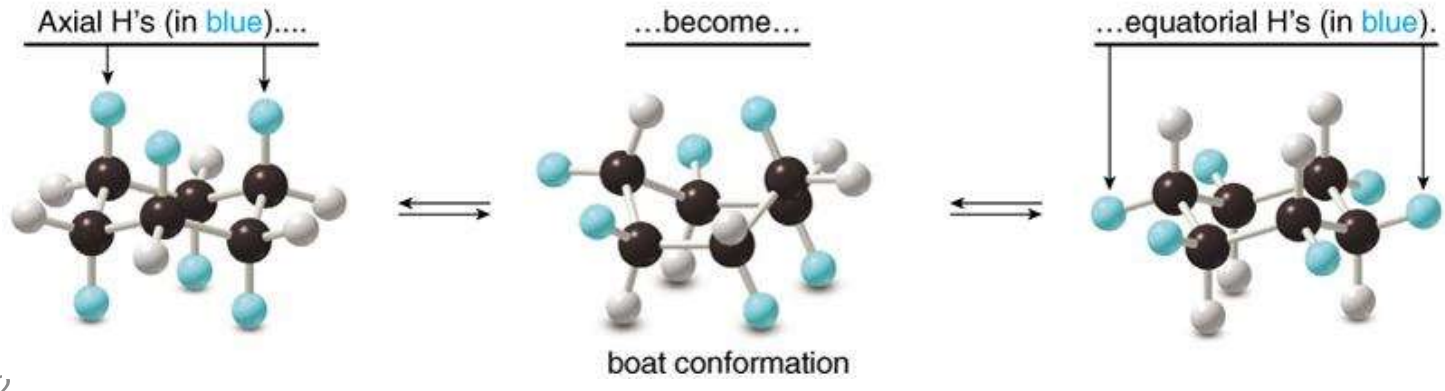




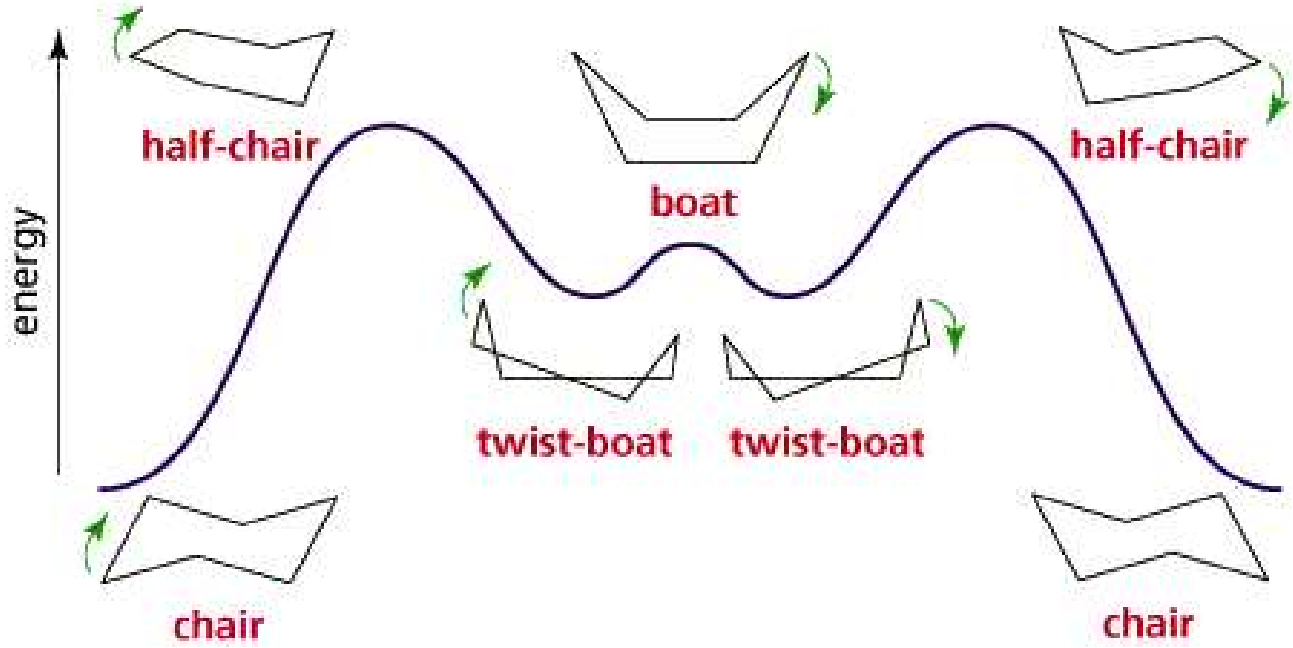
Ring-flipping

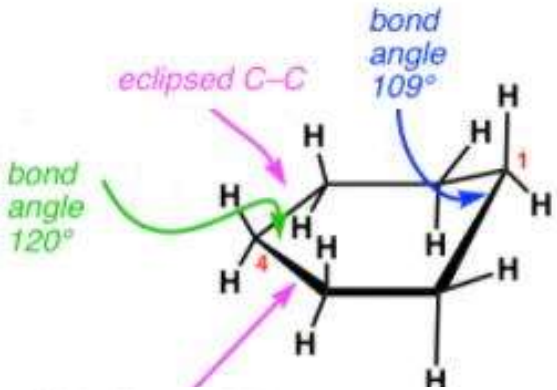
- *An important conformational change in cyclohexane involves "ring-flipping."*
- *As a result of a ring flip, the up carbons become down carbons, and the down carbons become up carbons.*
- *Axial and equatorial H atoms are also interconverted during a ring-flip. Axial 'H' atoms become equatorial H atoms, and equatorial H atoms become axial H atoms.*





Mechanism of Ring Flip

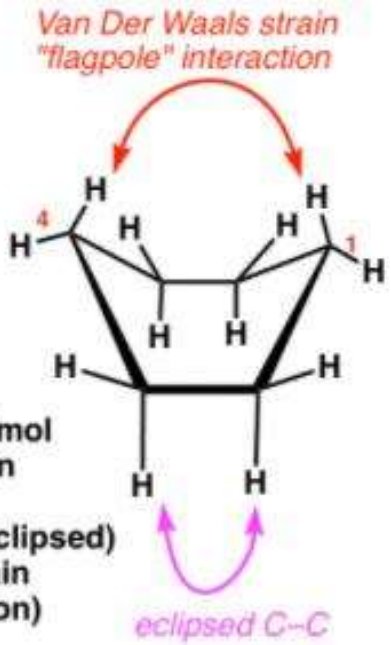




"Half chair"

Ring strain 10.8 kcal/mol

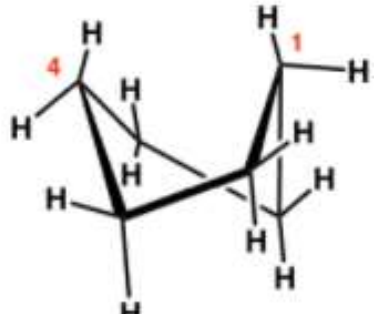
- some angle strain (120°)
- torsional strain (two C–C bonds fully eclipsed, two more partially eclipsed)



"Boat"

Ring strain 7.0 kcal/mol

- minimal angle strain
- torsional strain (some C–C bonds eclipsed)
- Van Der Waals strain ("flagpole" interaction)



"Twist Boat"

Ring strain 5.5 kcal/mol

- relief of Van Der Waals strain through twisting
- minimal angle strain
- torsional strain (some eclipsed C–C bonds)