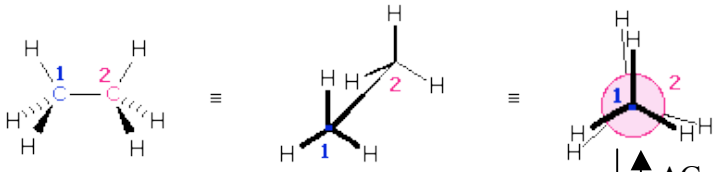
Conformations

- Different 3-D shapes a molecule can assume by rotation around single bonds.

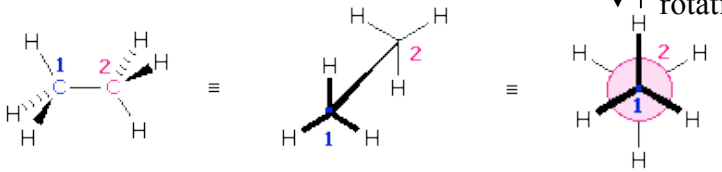
Eg) ethane – C_2H_6

Newman projection

Less stable Eclipsed Conformation



Most stable Staggered Conformation



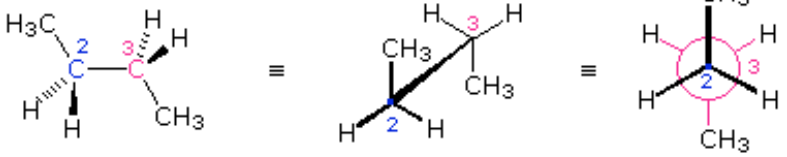
ΔG = 2.8 kcal/mol for rotation

- Rotation occurs rapidly at room temperature.
- Room temperature = ~15-20 kcal/mol of energy available.

Eg) n-butane (C_4H_{10}) – rotation around all bonds still very rapid

- most stable (most populated conformation) is called anti and has groups as far away as possible

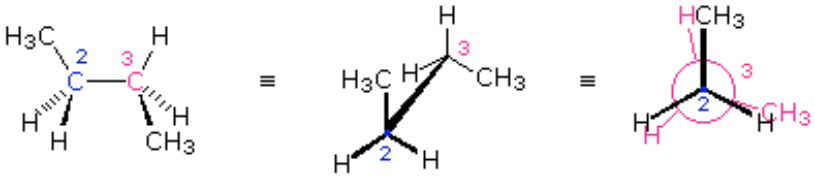
A



Anti Conformation

Most stable, staggered
Dihedral angle = 180°

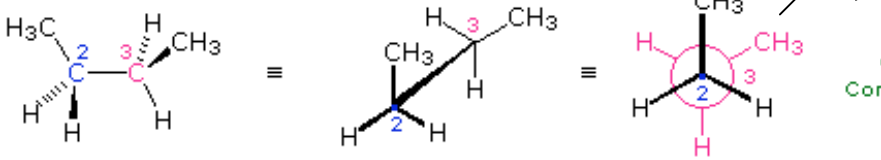
B



Eclipsed Conformation

Dihedral angle = 120°

C

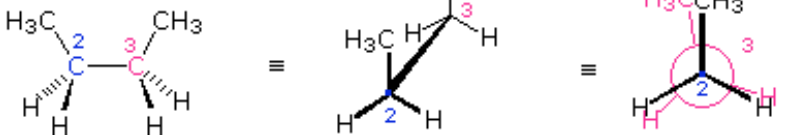


Repulsion = steric effect

Gauche Conformation

Not as stable as anti
Dihedral angle = 60°

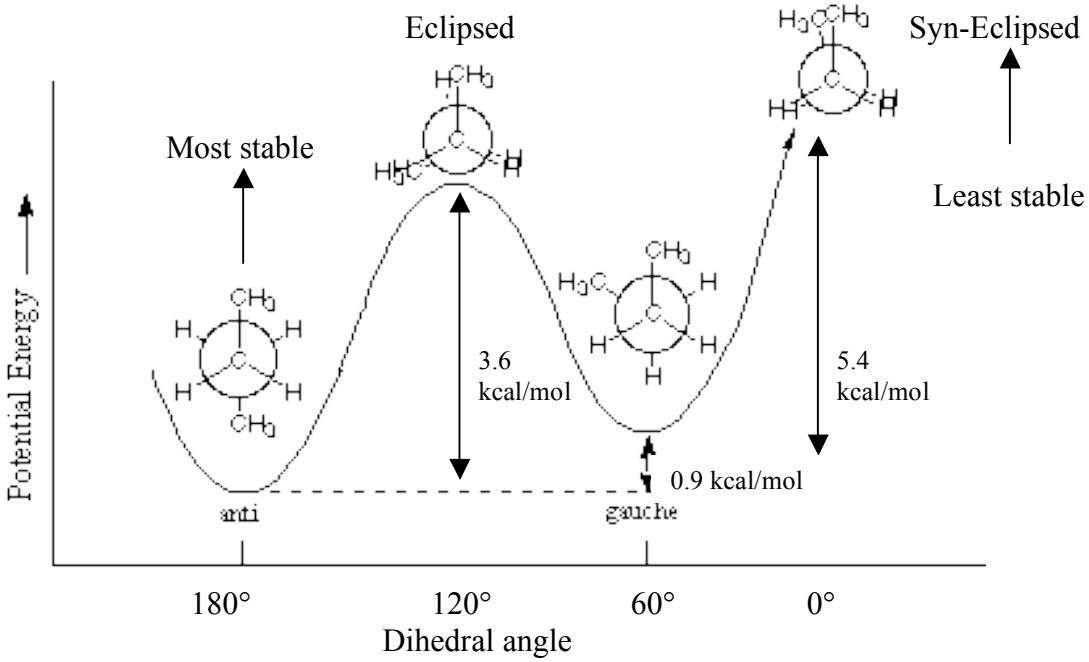
D



Eclipsed Conformation

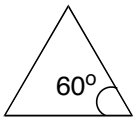
Least stable (syn)
Dihedral angle = 0°

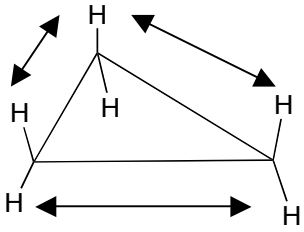
The dihedral angle is the angle between the two-methyl groups



Cycloalkane Conformations

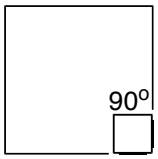
Eg) Cyclopropane –bond angle 60°



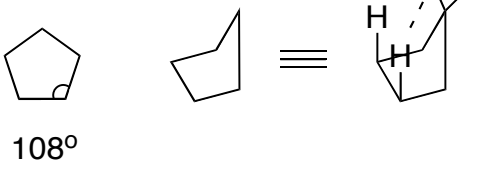


Eclipsing interactions

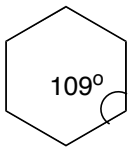
Eg) Cyclobutane – bond angle close to 90°



Eg) Cyclopentane – bond angles nominally 108°

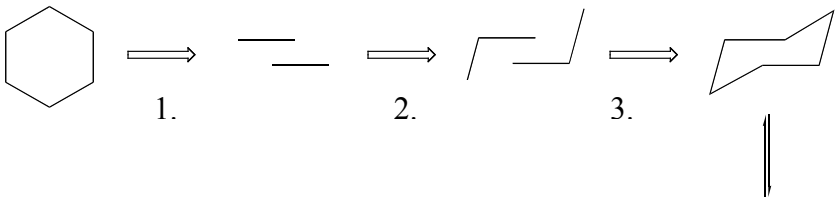


Eg) Cyclohexane – bond angles actually 109° not 120° as in flat hexagon

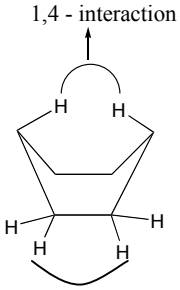


With envelope conformation there are
still bad H-H interactions.

Cyclohexane Conformations – How to draw:

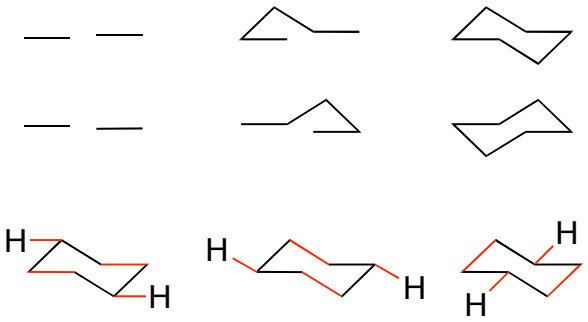


- Chair conformation (most stable)
- All adjacent hydrogen atoms are staggered

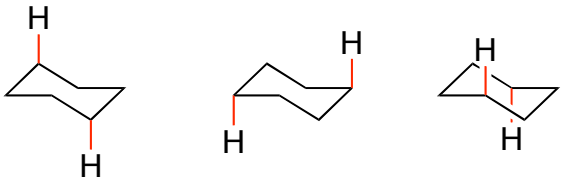


- Boat (least stable)
- many adjacent hydrogen atoms eclipsed
- 1,4 - interactions of two-hydrogens

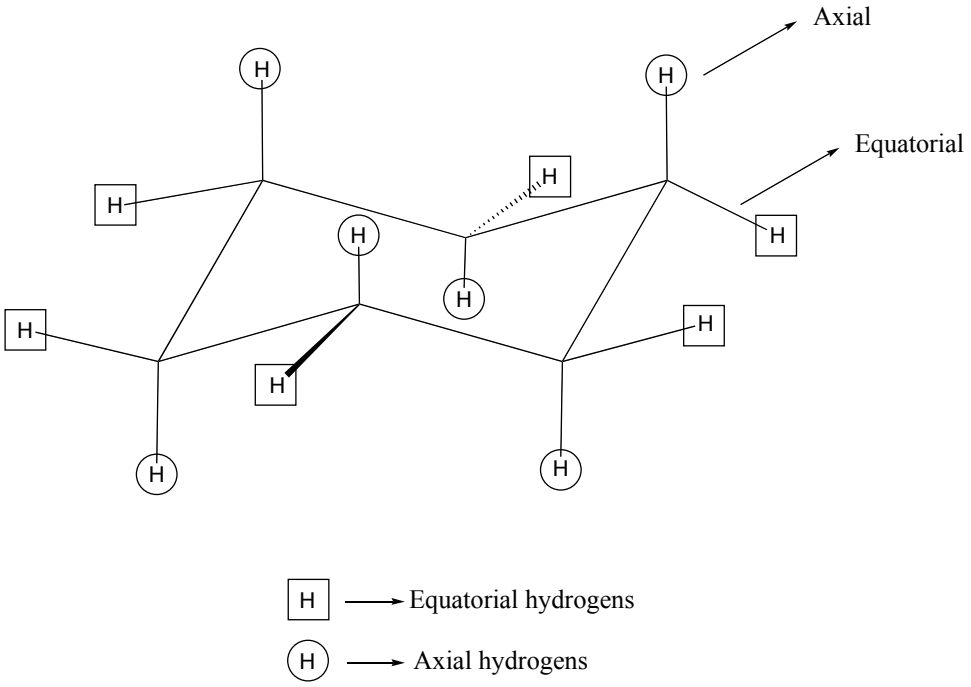
Another way to draw cyclohexane:



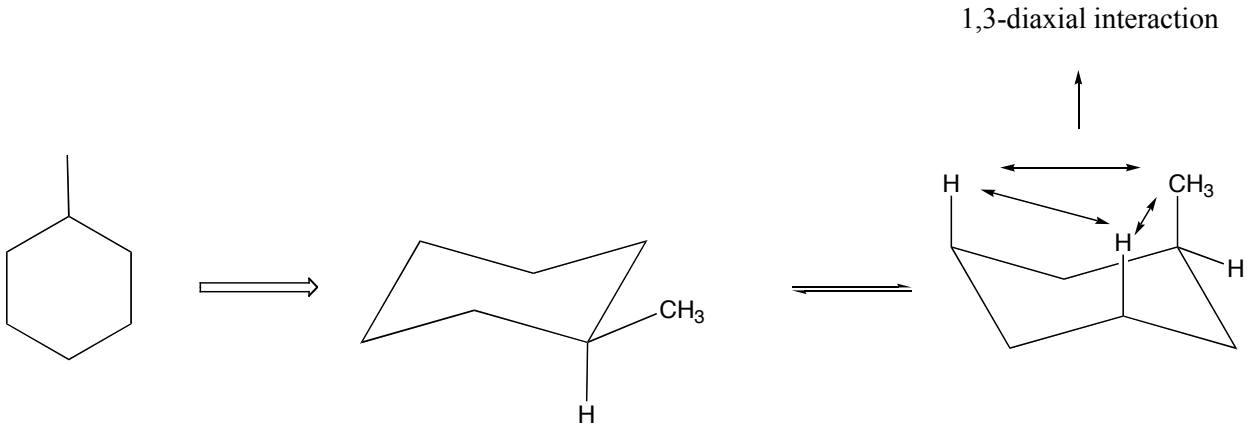
Parallel Lines in Equatorial Position



Vertical Lines in Axial Position



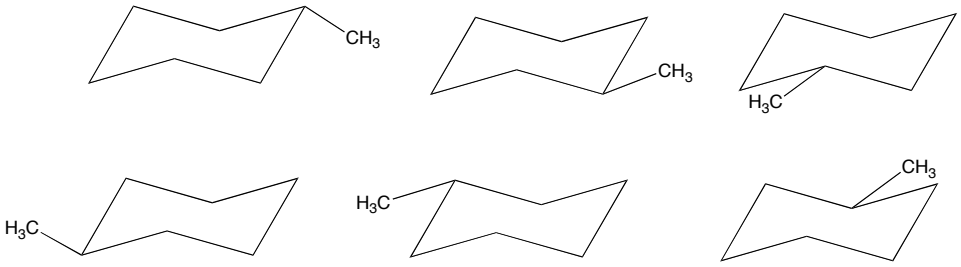
Substituted Cyclohexanes – Draw most stable conformation



- Largest (bulkiest group close to ring) group generally placed equatorial – otherwise get unfavorable 1,3-diaxial interactions

- 1,3-diaxial interaction (steric effect) makes this conformation less stable.

Most Stable Conformation of Methylcyclohexane – 6 drawings of same molecule below

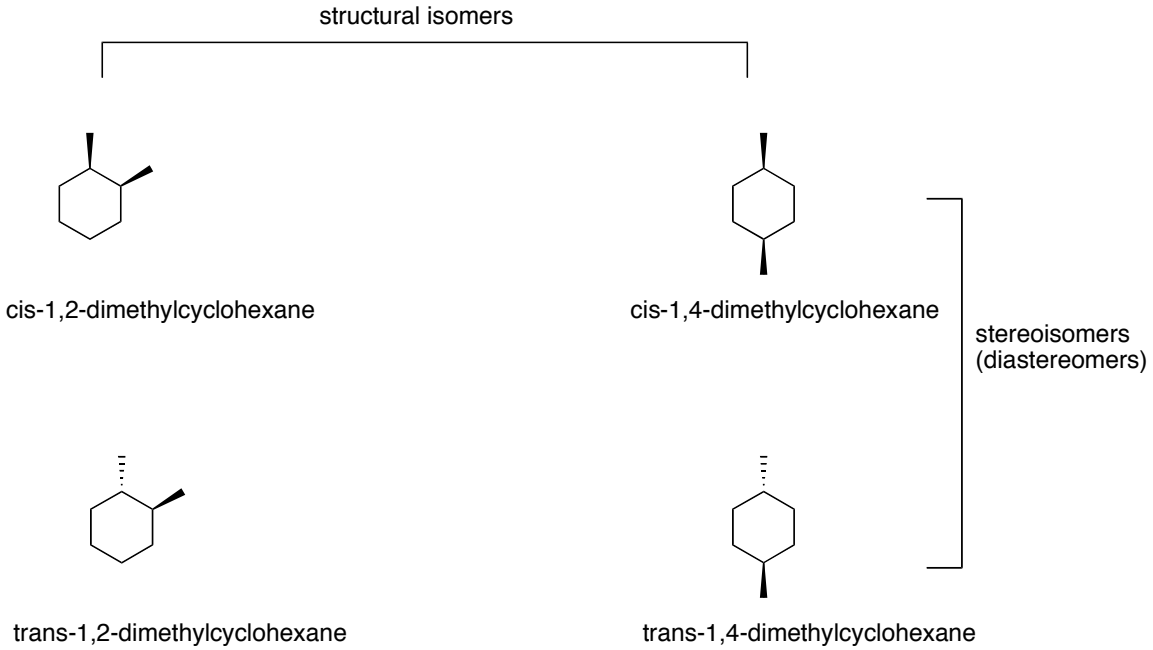


Polysubstituted cyclohexane

Isomers - different compounds with same molecular formula

Conformers – different shapes of the same molecule

Example: 1,2-dimethylcyclohexane and 1,4-dimethylcyclohexane



Diastereomers have different chemical and physical properties and they can be converted to each other just by chemical reactions.

Trans (1,4) conformation: