Review:

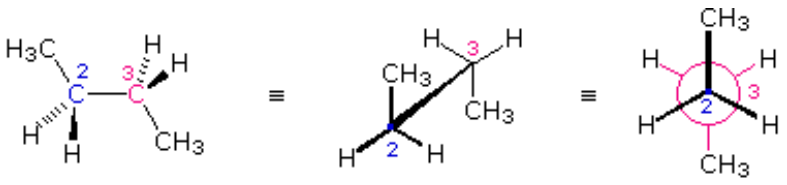
Conformations – Different shapes a single molecule may assume via rotation around single bonds
Isomers - Different compounds with same molecular formula – 2 basic types
1. Structural/constitutional isomers
   – Compounds with same molecular formula
2. Stereoisomers – Same connectivity but different 3-D structure – 2 sub-types
   (a) diastereomers/diastereoisomers (eg. *cis*/*trans*)
   (b) enantiomers (non-superimposable mirror images of same molecule).

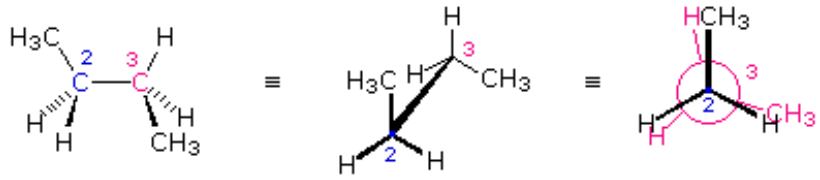
*Do not confuse conformers (single compund shapes) with isomers (different compounds with same molecular formula)

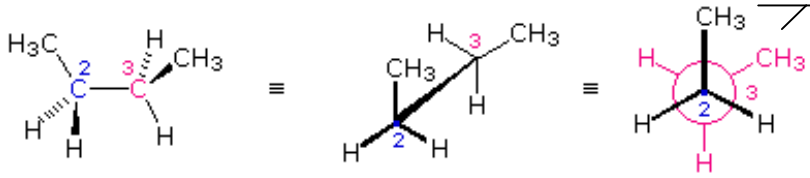
n-butane (C_4H_{10})

Rotation around all bonds still very rapid

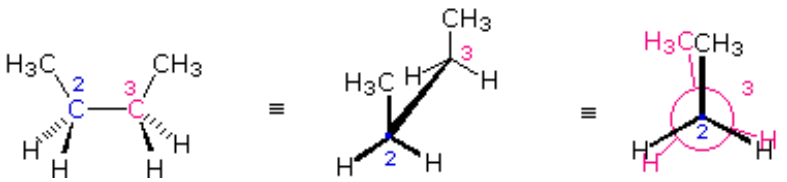
- Most stable (most populated conformation) is called anti and has groups as far away as possible

A  Anti Conformation — Most stable, staggered Dihedral angle = 180°

B  Eclipsed Conformation — Dihedral angle = 120°

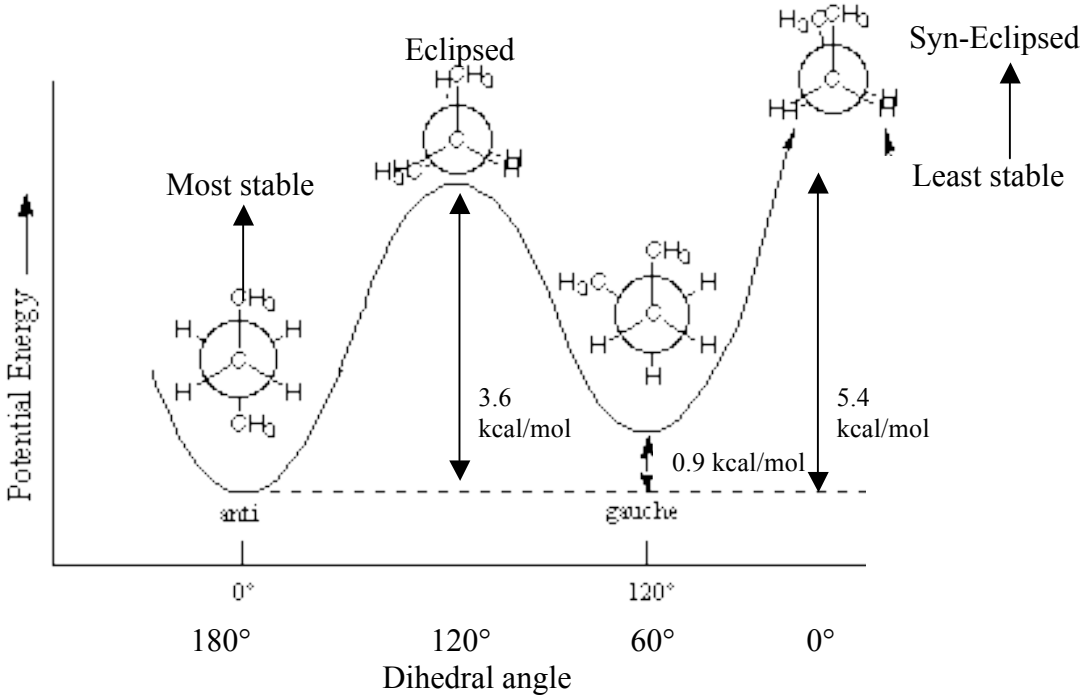
C  Repulsion = steric effect

Gauche Conformation — Not as stable as anti Dihedral angle = 60°

D  Eclipsed Conformation — Least stable (syn) Dihedral angle = 0°

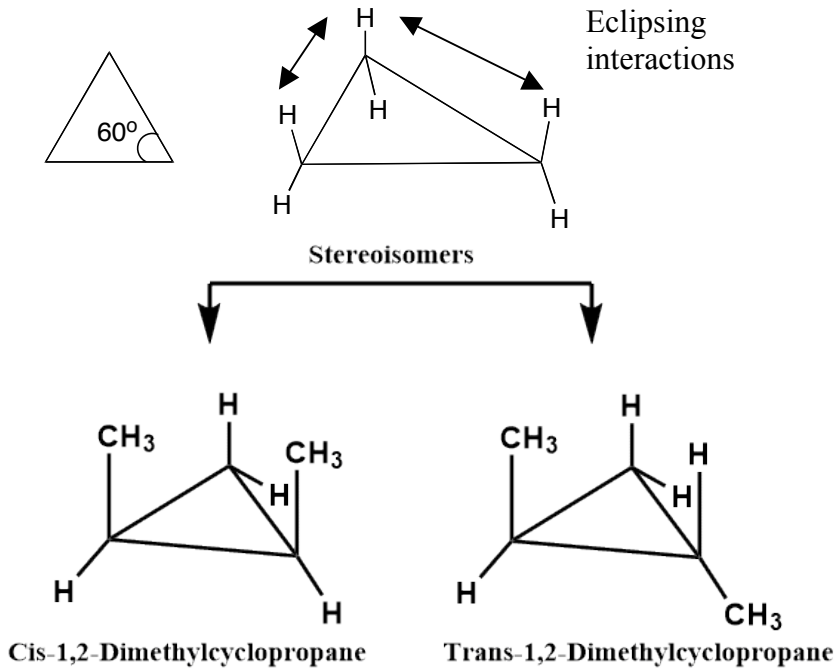
Energy diagram

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

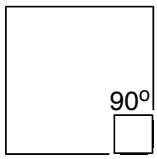


Cycloalkane Conformations

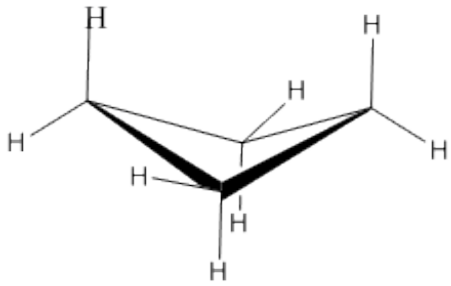
Cyclopropane –bond angle 60^{o} – relatively rigid structure



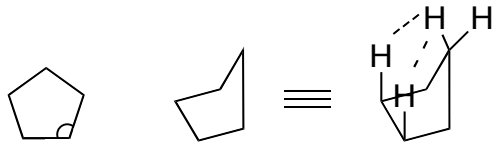
Cyclobutane – bond angle close to 90^o – does have some flexibility



3D structure

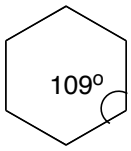


Cyclopentane – bond angles nominally 108^o – more flexible than cyclobutane

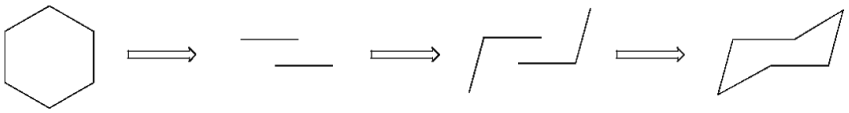


108°

Cyclohexane – bond angles actually 109^o, not 120^o as in flat hexagon

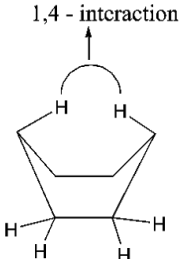


Cyclohexane Conformations – How to draw:



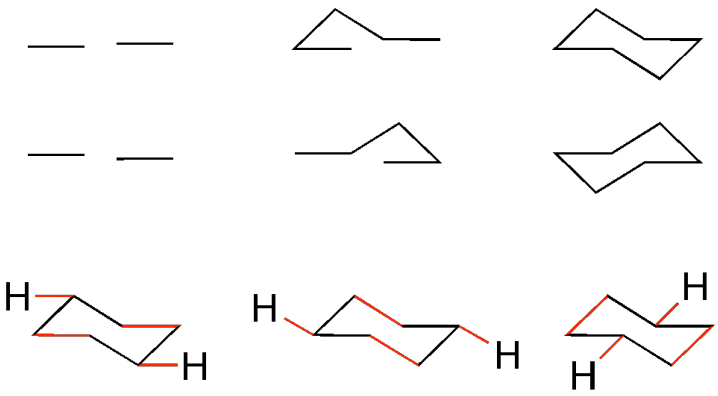
- Chair conformation (most stable)
- All adjacent hydrogen atoms are staggered

1,4 - interaction

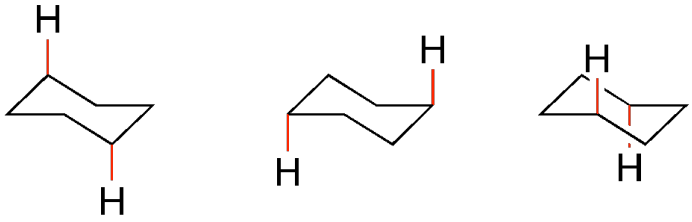


- Boat (least stable)
- many adjacent hydrogen atoms eclipsed
- 1,4 - interactions of two-hydrogens

Another way to draw cyclohexane:

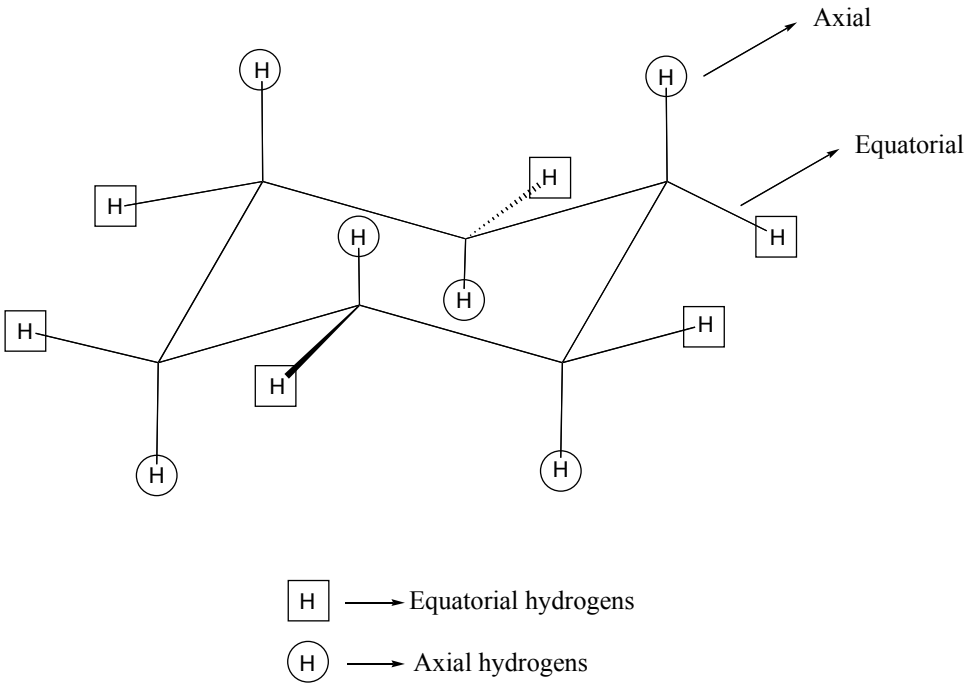


Parallel Lines in Equatorial Position

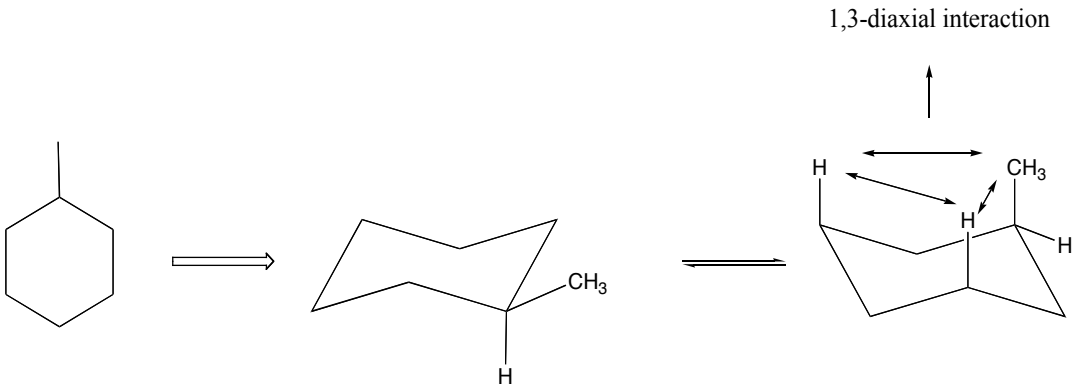


Vertical Lines in Axial Position

Cyclohexane Conformations Axial vs Equatorial positions



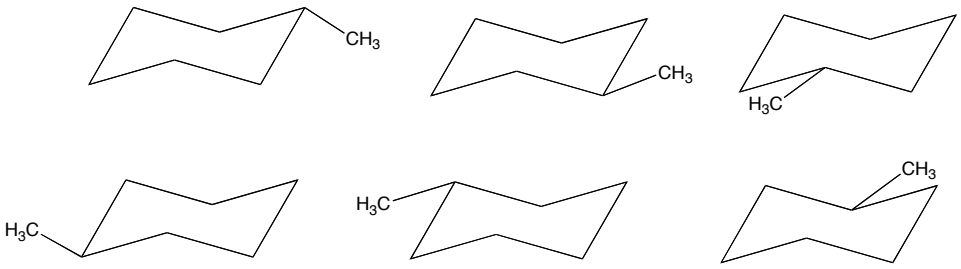
Substituted Cyclohexanes – Draw most stable conformation



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

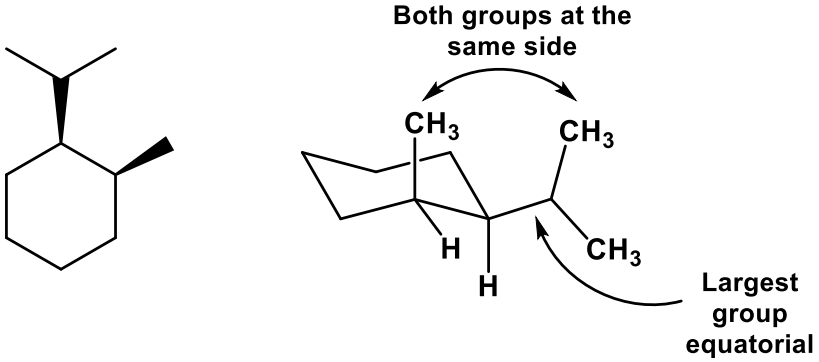
- 1,3-diaxial interaction (steric effect) makes this conformation less stable.

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

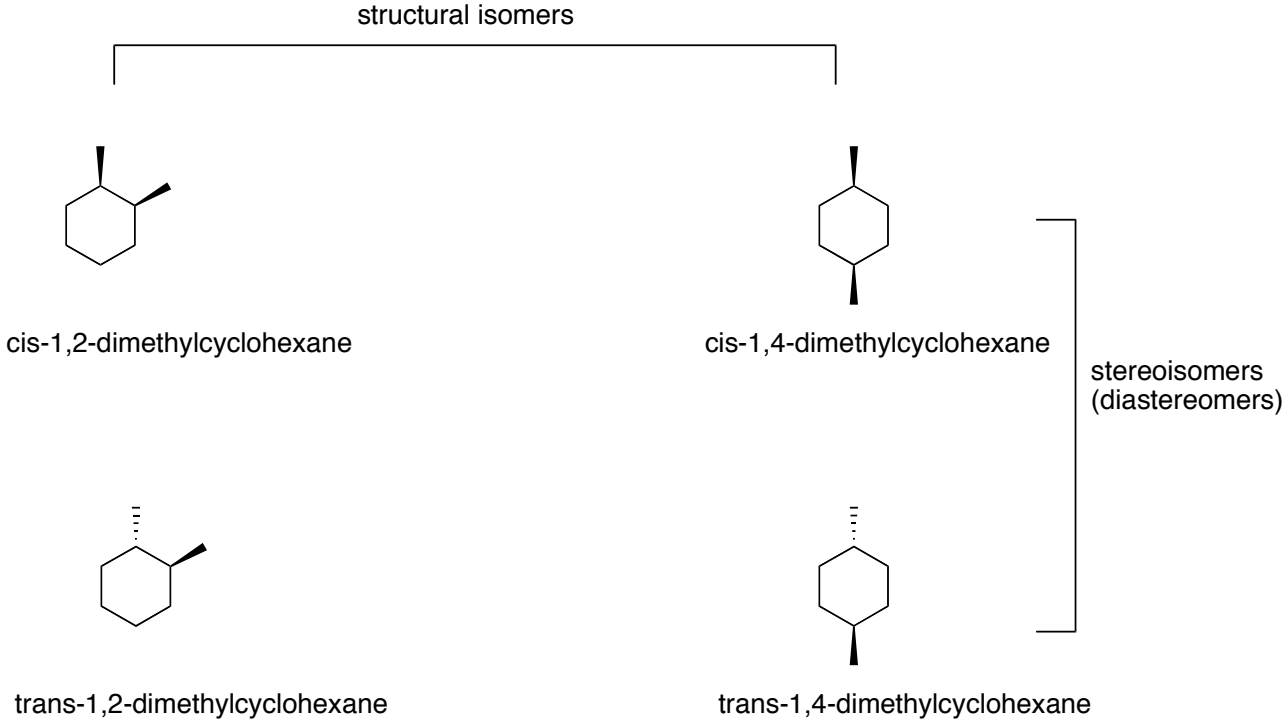


Polysubstituted cyclohexanes

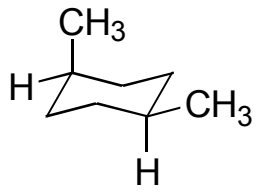
Example: cis-1-isopropyl-2-methylcyclohexane



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

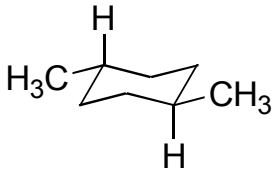


Example: cis-1,4-dimethylcyclohexane:



Cis-1,4-Dimethyl Cylcohexane

Example: trans-1,4-dimethylcyclohexane:



Trans-1,4-Dimethyl Cylcohexane