## Conformations:

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

Eg) ethane $-\mathrm{C}_{2} \mathrm{H}_{6}$
Newman projection

Less stable
Eclipsed Conformation


$-$


Most stable
Staggered Conformation


$\equiv$


- Rotation occurs rapidly at room temperature.
- Room temperature $=\sim 15-20 \mathrm{kcal} / \mathrm{mol}$ of energy available.
$\mathrm{Eg})$ n-butane $\left(\mathrm{C}_{4} \mathrm{H}_{10}\right)$ - rotation around all bonds still very rapid
- most stable (most populated conformation) is called anti and has groups as far away as possible




## Cycloalkane Conformations

Eg) Cyclopropane -bond angle $60^{\circ}$



Eg) Cyclopentane - bond angles nominally $108^{\circ}$


Eg) Cyclobutane - bond angle close to $90^{\circ}$


Eg) Cyclohexane - bond angles actually $109^{\circ}$ not $120^{\circ}$ as in flat hexagon


Cyclohexane Conformations - How to draw and what they mean


$\mathrm{H} \longrightarrow$ Equatorial hydrogens
H $\longrightarrow$ Axial hydrogens

Substituted Cyclohexanes - Draw most stable conformation


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

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


Substituted Cyclohexanes - draw most stable conformation
Eg \#1 - cis-1,4-dimethylcyclohexane


1,4 - dimethylcyclohexane

Eg \#2 - a trans-1,4-disubstituted cyclohexane


Generally, draw a chair, add the most bulky group at one end in equatorial position. The determine where the next group should go (which carbon and whether axial or equatorial) remember: the given flat drawing geometry determines the 3D orientation

Eg. \# 3 - A poly-substituted cyclohexane - most stable conformation?
First draw chair conformation, then place bulkiest (largest) group (e.g. t-butyl) equatorial at one end.
Then work on which orientation the remaining substituents have based on the given "flat" geometry picture. So for position 2, the methyl must be below the hydrogen at the same carbon because at position 1 the t-butyl group is above the hydrogen at position 1 and trans geometry (opposite sides) is required for the relationship of the two groups (methyl and t-butyl). Etc.


Other ring systems - see additional graphics pages at our web site

Norbornane
Adamantane
(part of diamond structure



Adamantane


Steroid

cholesterol

