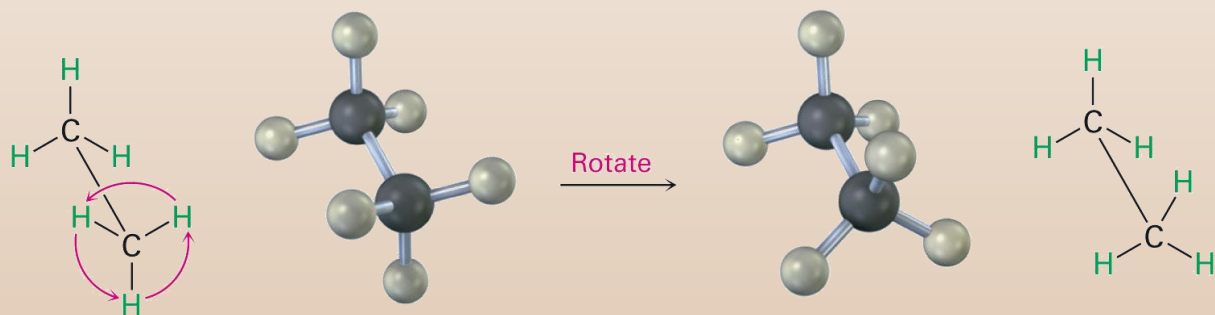


Alkanes - 4 - Conformations

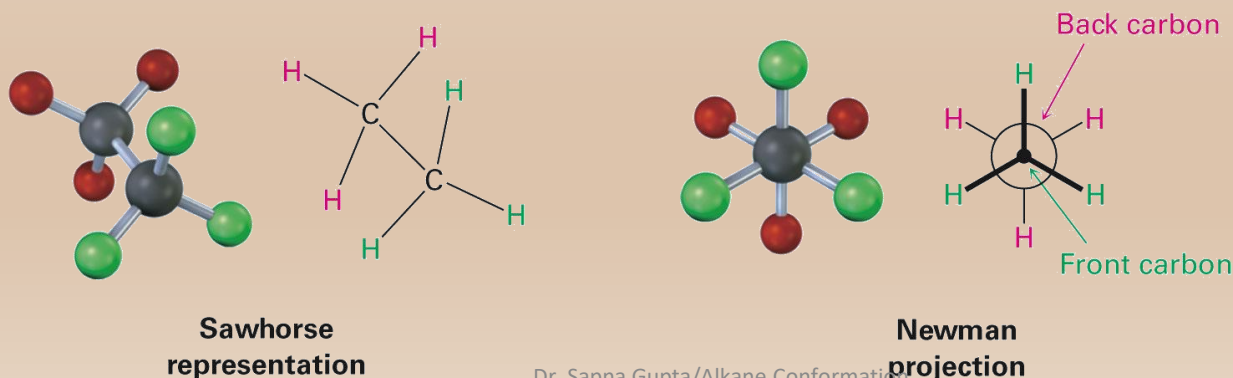
Dr. Sapna Gupta

Conformation

- Different representation of molecules because of rotation around single bonds
- All sp^3 bonds in straight chain alkanes can rotate but in cycloalkanes rotation is not possible (hence the cis and trans isomers possible)

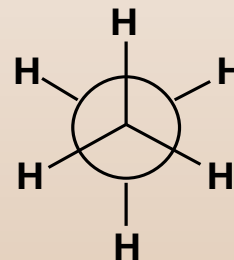
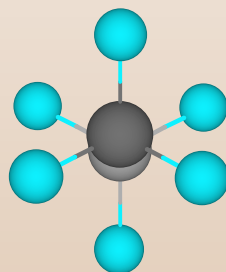
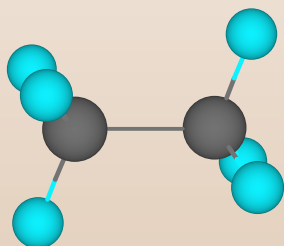


- Fisher (sawhorse) projection and Newman projections

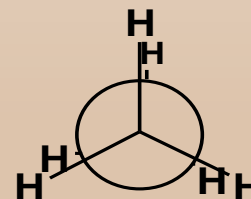
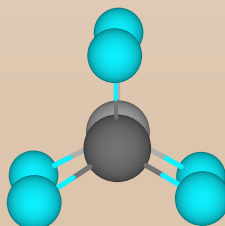
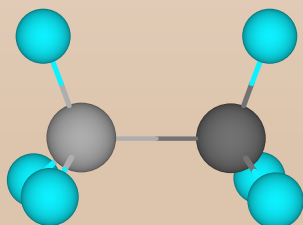


Torsional Strain

- Torsional strain arises when nonbonded atoms separated by three bonds are forced from a **staggered** conformation to an **eclipsed** conformation.
- **Staggered**- most stable: all 6 C-H bonds are as far away as possible

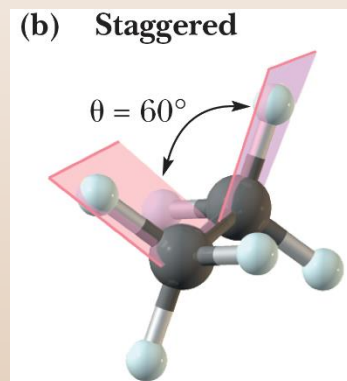
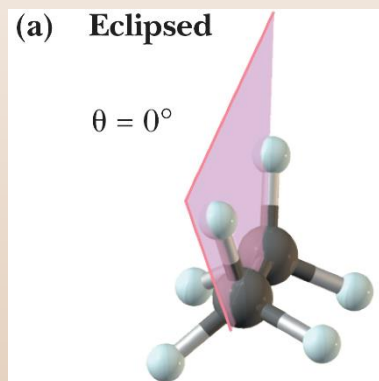


- **Eclipsed**- least stable: all 6 C-H bonds are as close as possible to each other



Conformations - Terminology

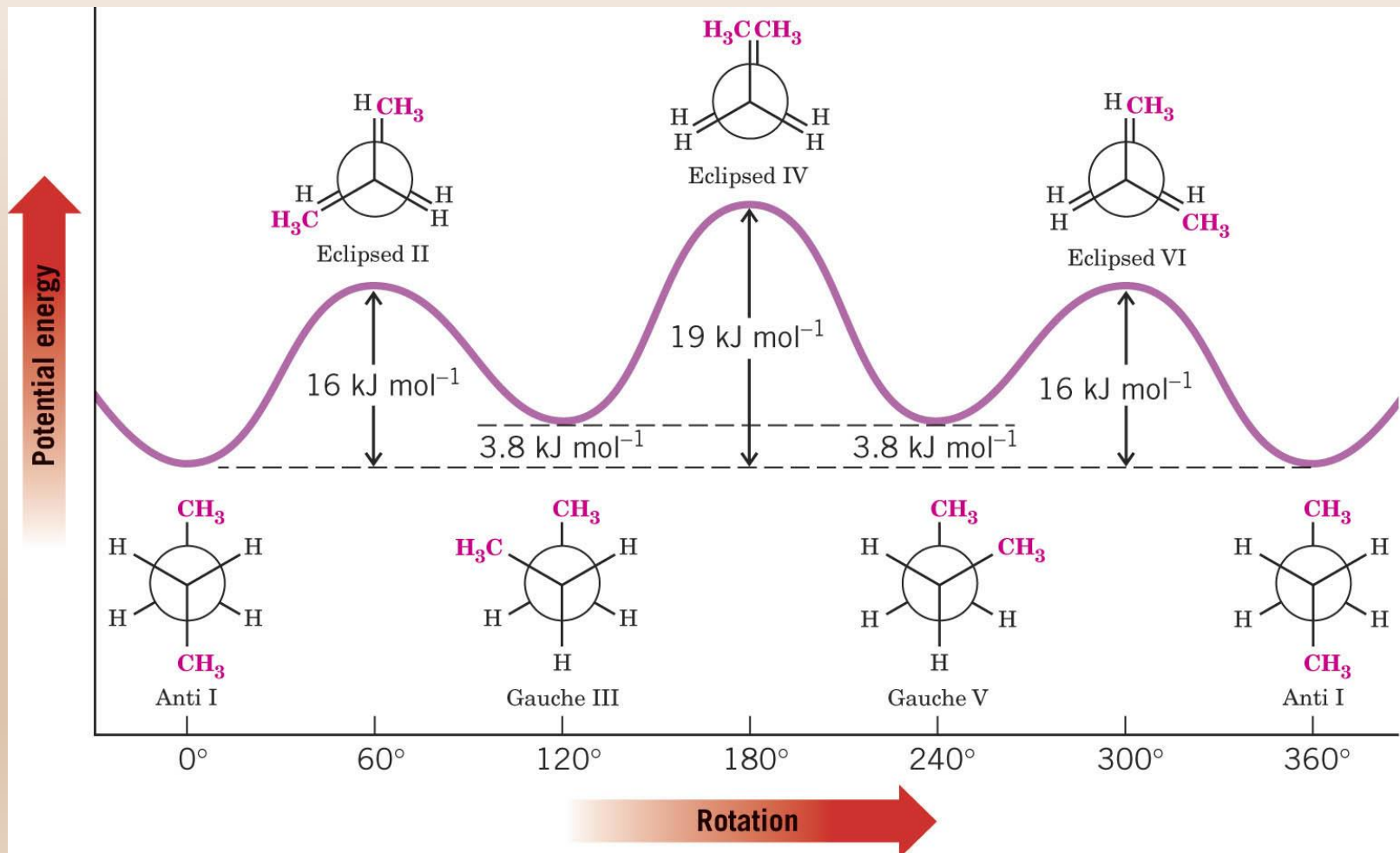
- **Dihedral angle** Θ (Greek theta): The angle created by two intersecting planes.



- **Steric strain** (nonbonded interaction strain): The strain that arises when nonbonded atoms separated by four or more bonds are forced closer to each other than their atomic (contact) radii will allow.
- **Angle strain**: Strain that arises when a bond angle is either compressed or expanded compared to its optimal value.

Conformations

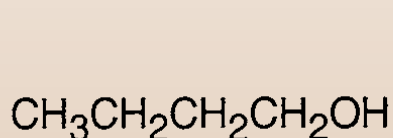
The energy of butane as a function of the dihedral angle about the bond between carbons 2 and 3.



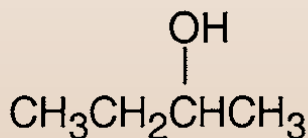
Solved Example

Draw as many compounds as you can that are alcohols with the formula, C_4H_8O . Draw the conformation of one of the constitutional isomers.

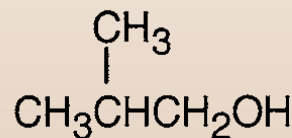
Answer:



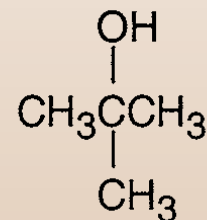
1-butanol



2-butanol



isobutyl alcohol

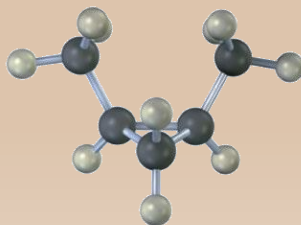
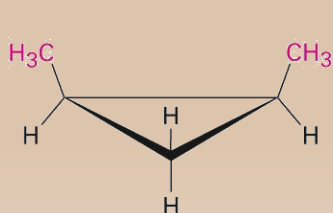


tert-butyl alcohol

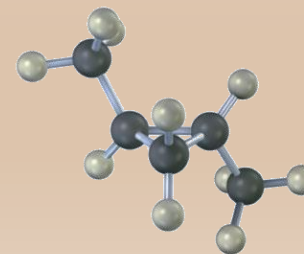
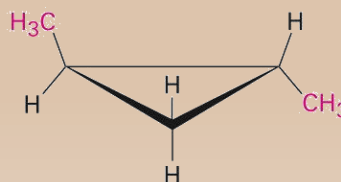
- Chose any of the above structures. Use C2 and C3 to use for looking at conformers. C1 will usually not exhibit so much steric and torsional strain because one carbon will have only hydrogens which are too small of atoms to have any strains.

Cycloalkanes

- **Angle strain** is caused by bond angles different from 109.5° (should be 109° because in single bond carbons are sp_3 hybridized)
- **Tortional strain** is caused by eclipsing C-H bonds on adjacent carbons
- **Steric strain** is due to close proximity of atoms or groups.
- Cycloalkanes are less flexible than open-chain alkanes
- Much less conformational freedom in cycloalkanes
- Because of their cyclic structure, cycloalkanes have 2 faces: “top” face
“bottom” face
- Therefore, **isomerism** is possible in substituted cycloalkanes
- There are two different 1,2-dimethylcyclopropane isomers – cis and trans



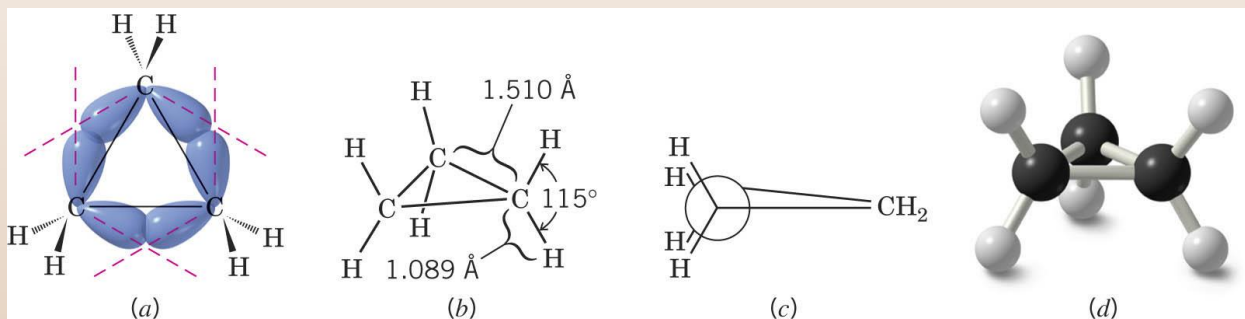
cis-1,2-Dimethylcyclopropane



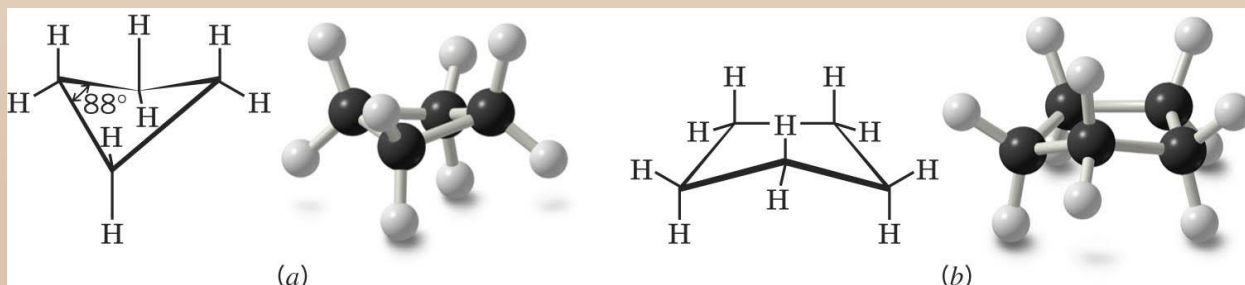
trans-1,2-Dimethylcyclopropane

Cyclopropane and Cyclobutane

- Cyclopropane has both angle and torsional strain. Cyclopropane is also a planar structure. Bond angle is 60° .

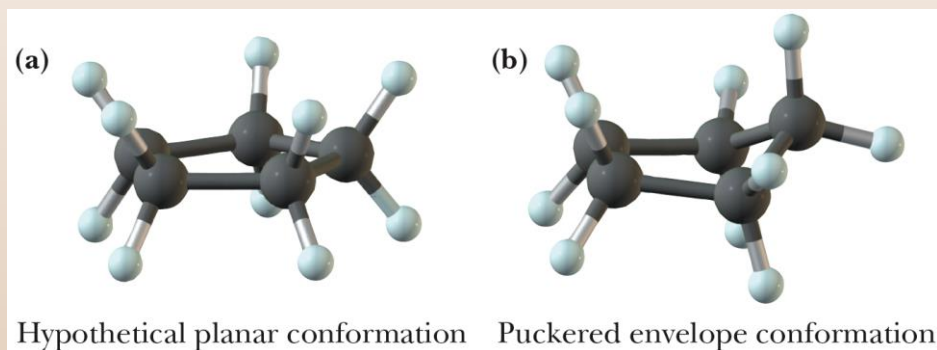


- Cyclobutane has more angle strain. Bond angle is 90°

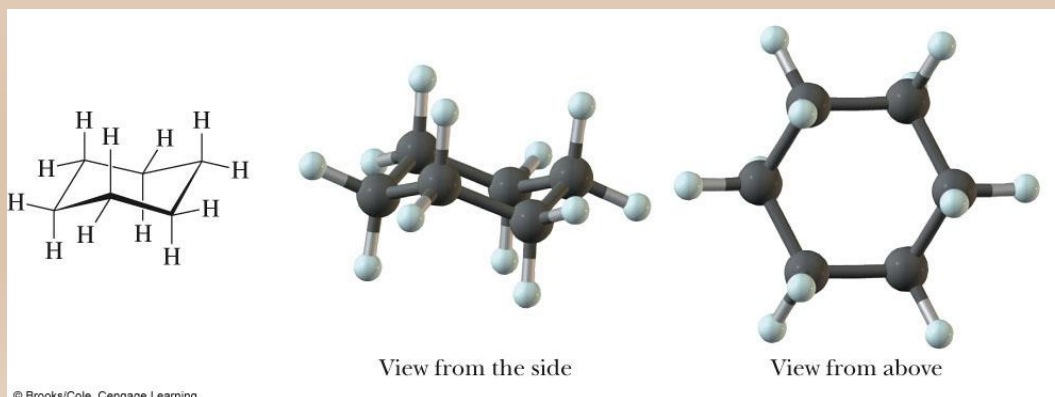


Cycloalkanes...

- Cyclopentane is slightly bent (puckered) which reduces the torsional strain. Bond angle is 108°

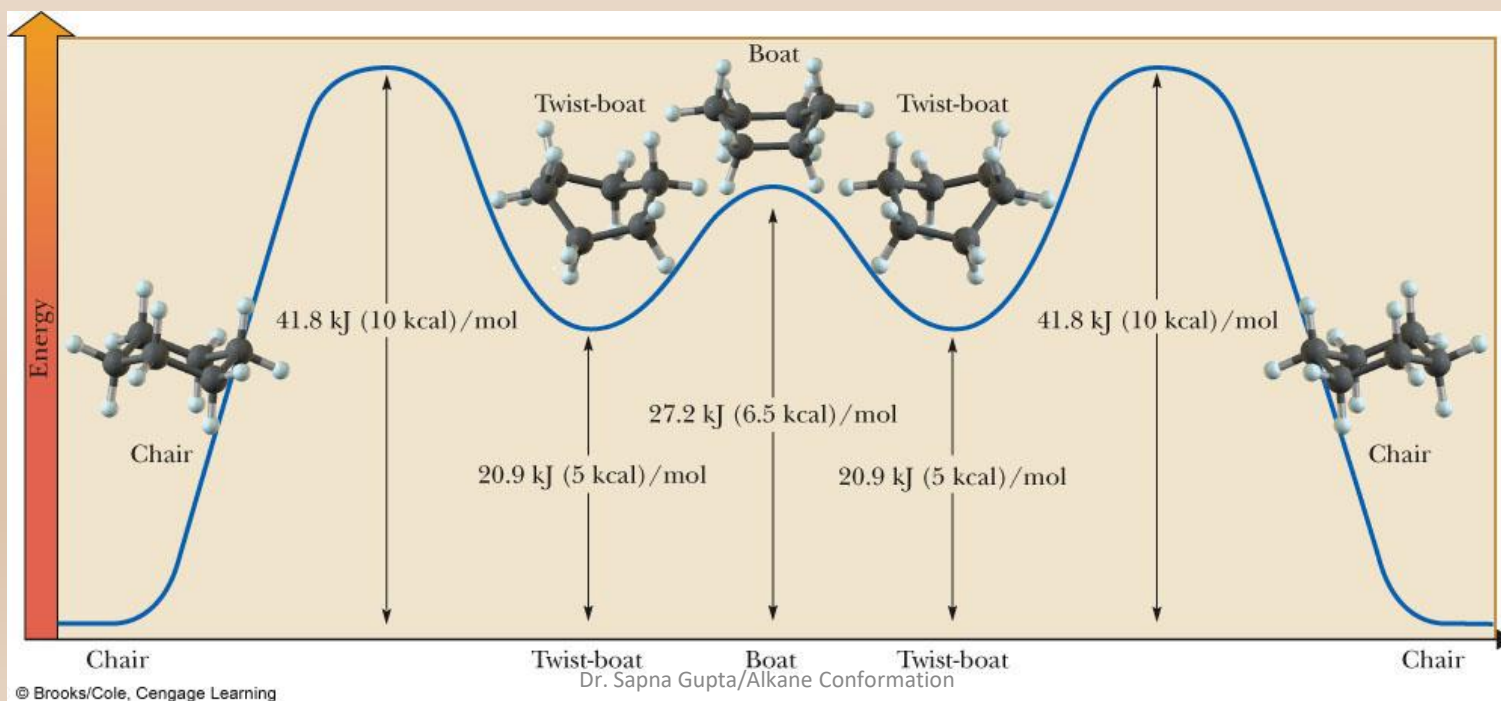


- Cyclohexane has the most stable ring. Bond angle is 120°



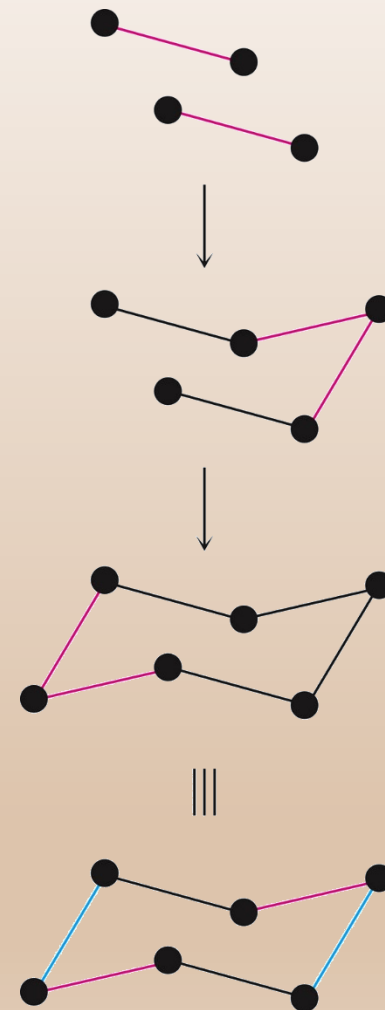
Conformation of Cyclohexane

- Remember bonds in cyclic compounds cannot rotate but they can still move up or down within certain limits.
- Cyclohexane ring is the most stable of rings and has two main conformers, chair and boat. (boat is not stable)
- The chair conformation is more stable and can further have two conformations when it flips to the other conformer.



How to Draw Cyclohexane

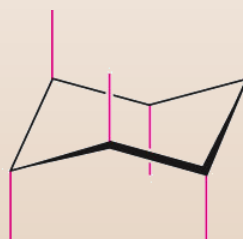
- Step 1** Draw two parallel lines, slanted downward and slightly offset from each other. This means that four of the cyclohexane carbons lie in a plane.
- Step 2** Place the topmost carbon atom above and to the right of the plane of the other four, and connect bonds.
- Step 3** Place the bottommost carbon atom below and to the left of the plane of the middle four, and connect the bonds. Note that the bonds to the bottommost carbon atom are parallel to the bonds to the topmost carbon.



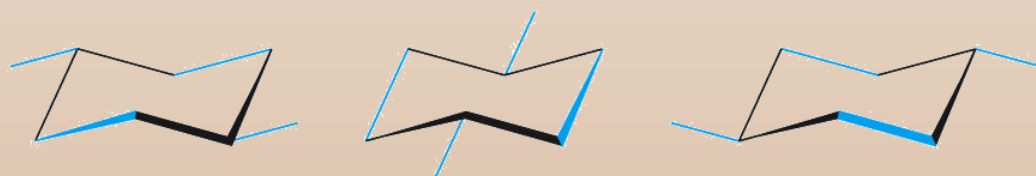
Drawing the Axial and Equatorial Hydrogens

Keep an eye on just one color at a time and see how the location changes

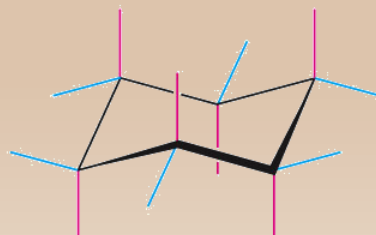
Axial bonds: The six axial bonds, one on each carbon, are parallel and alternate up-down.



Equatorial bonds: The six equatorial bonds, one on each carbon, come in three sets of two parallel lines. Each set is also parallel to two ring bonds. Equatorial bonds alternate between sides around the ring.

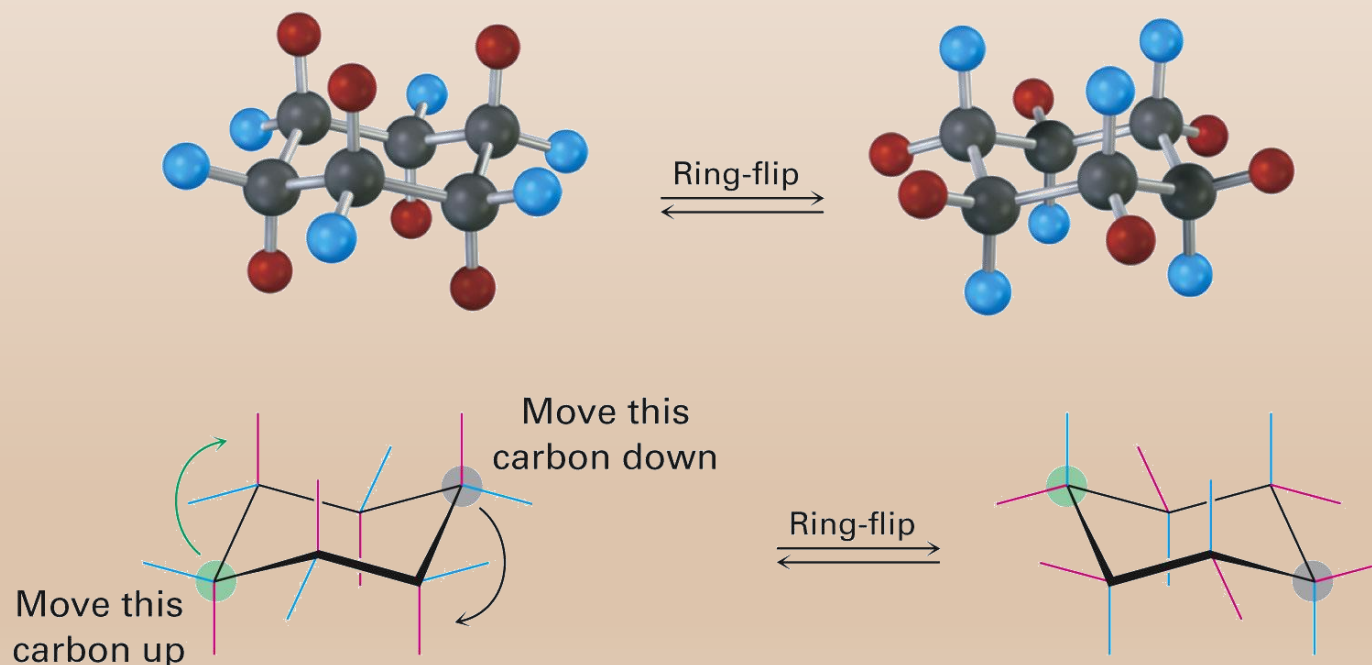


Completed cyclohexane



Conformation (ring flip) of Cyclohexane

- Chair conformations readily interconvert, resulting in the exchange of axial and equatorial positions by a **ring-flip**
- See a YouTube video here to see the ring flip: [LINK](#)
- See another one here....[LINK](#)



Axial and Equatorial Relationships in Disubstituted Cyclohexanes

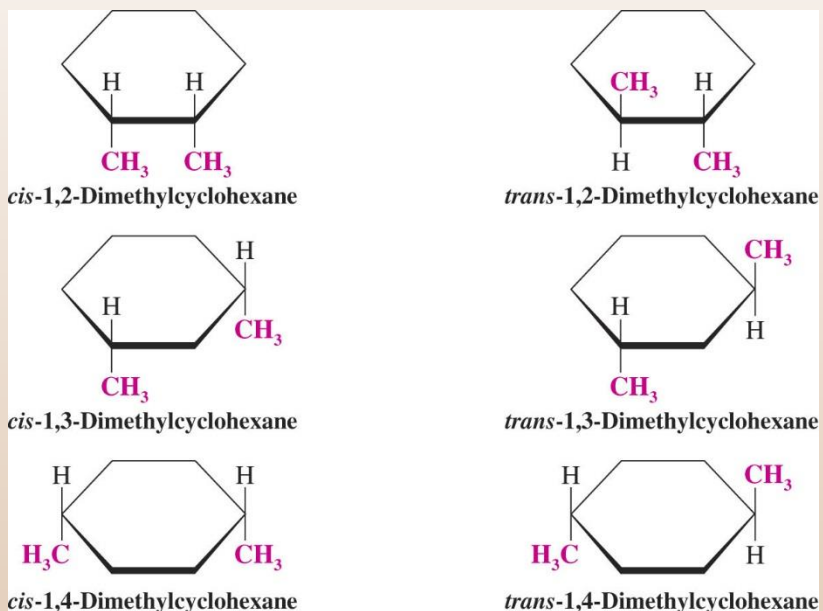
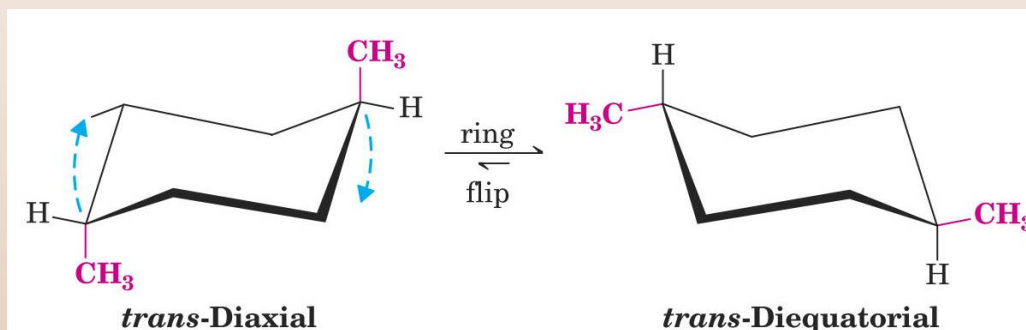


Table 4.2 Axial and Equatorial Relationships in Cis- and Trans-Disubstituted Cyclohexanes

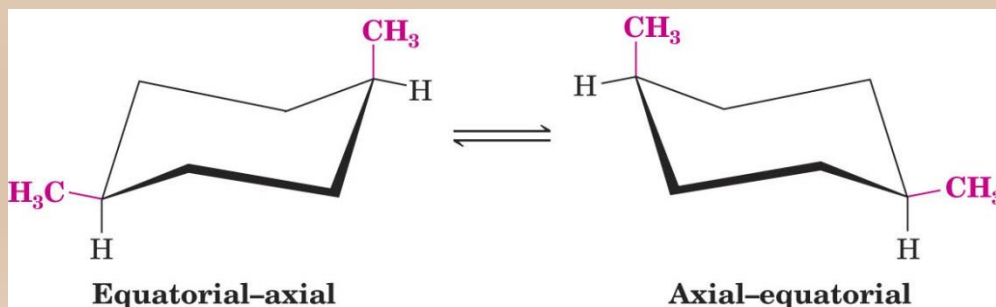
Cis/trans substitution pattern	Axial/equatorial relationships		
1,2-Cis disubstituted	a,e	or	e,a
1,2-Trans disubstituted	a,a	or	e,e
1,3-Cis disubstituted	a,a	or	e,e
1,3-Trans disubstituted	a,e	or	e,a
1,4-Cis disubstituted	a,e	or	e,a
1,4-Trans disubstituted	a,a	or	e,e

Trans-1,4-dimethylcyclohexane

- *Trans*-1,4-dimethylcyclohexane prefers a *trans*-diequatorial conformation



- *Cis*-1,4-dimethylcyclohexane exists in an axial-equatorial conformation (the only ones possible)



Key Words/Concepts

- Conformation
- Anti
- Gauche/staggered
- Eclipsed
- Torsional strain
- Angle strain
- Steric strain (steric hindrance)
- Cis and trans isomers (geometric isomers)
- Chair conformation
- Equatorial and axial substituents