Cyclic Alkane Conformers

UCI Chem 51A
Dr. Link

Goals

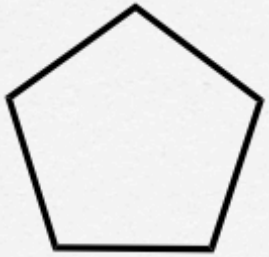
- After this lesson you should be able to
  - Identify the types of strain present in different cycloalkanes
  - Draw both chair conformers for cyclohexane
  - Draw chair conformers for substituted cyclohexane derivatives
  - Perform "chair flips" for cyclohexane derivatives
  - Distinguish between relative energies for different conformers for cyclohexane derivatives & explain the cause of the energy difference

Cyclic Alkanes Review

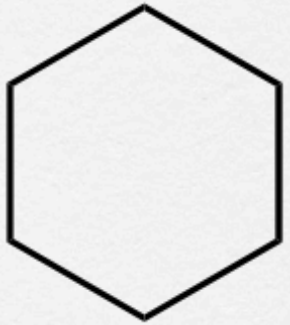
C_nH_{2n}

cyclopropane

cyclobutane

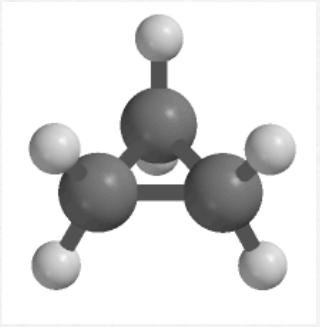


cyclopentane

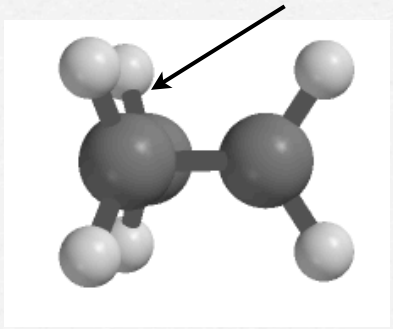


cyclohexane

Cyclopropane & Cyclobutane

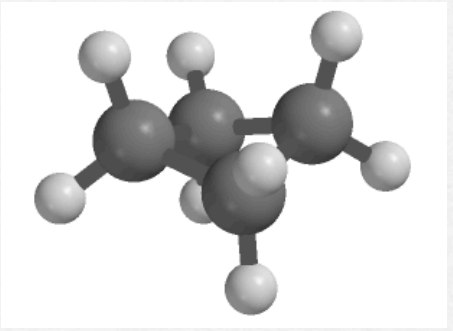


top view



side view

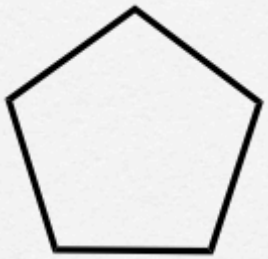
angle + torsional =

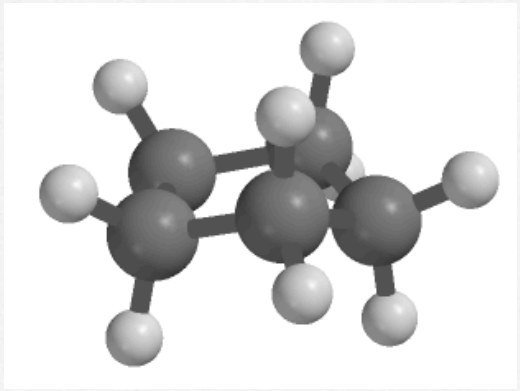


"butterfly"
not quite eclipsing

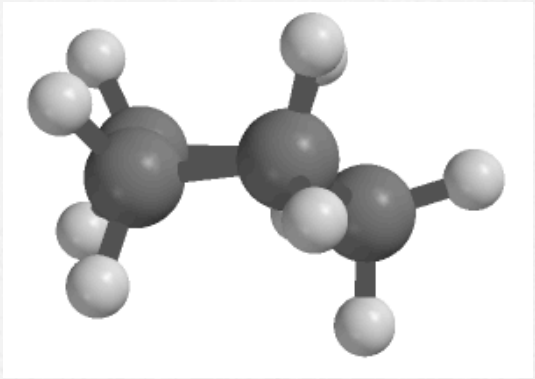
angle + torsional =

Cyclopentane



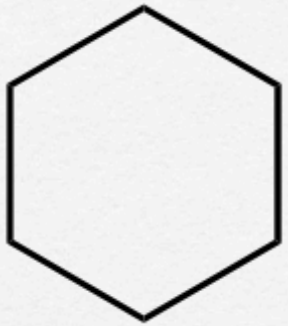


envelope conformer

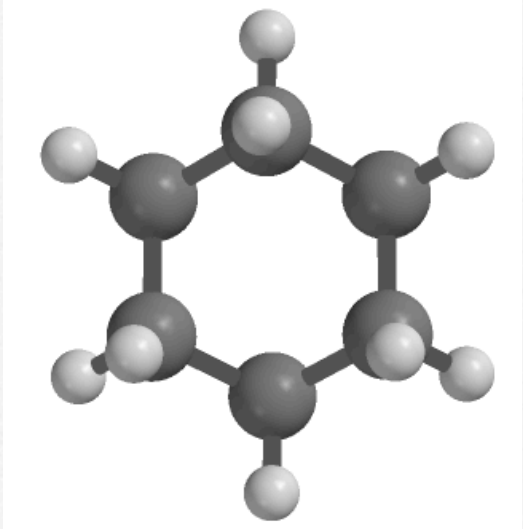


side view
eclipsing interactions

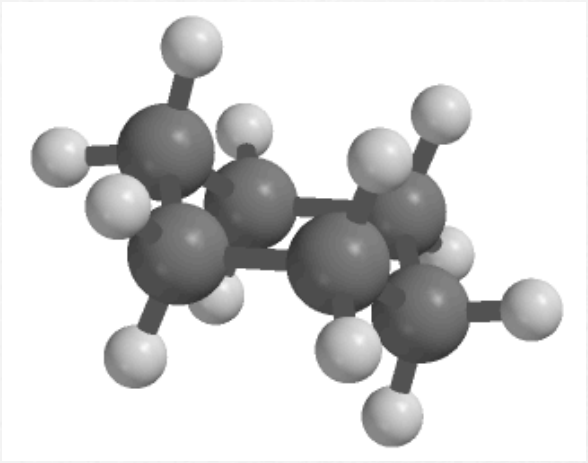
Cyclohexane



~120°?



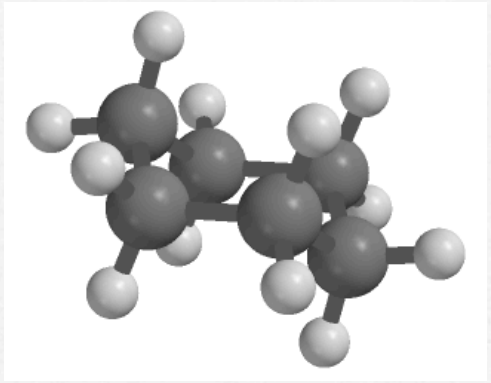
Top view



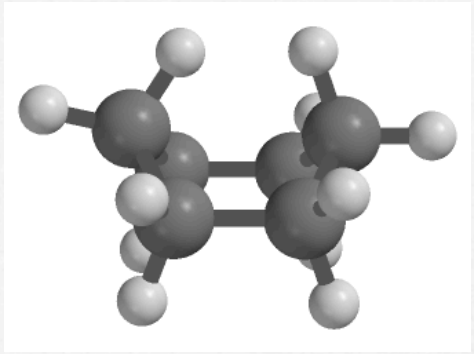
Side view

Not Planar!

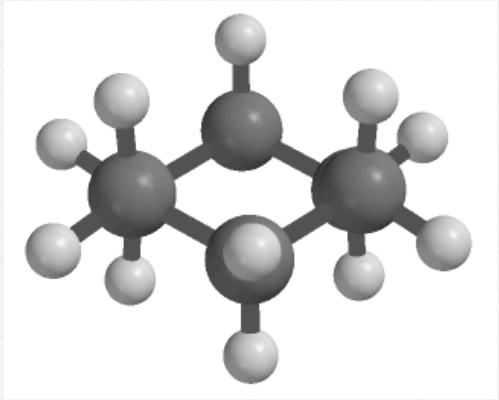
Chair Vs. Boat

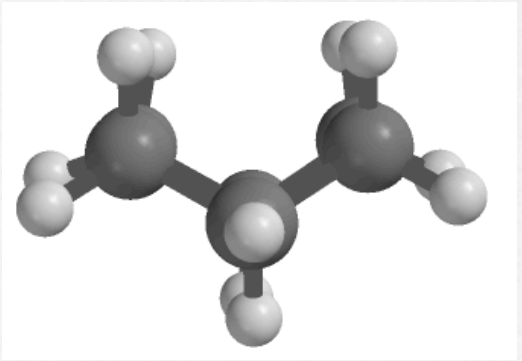


chair 0 kcal/mol

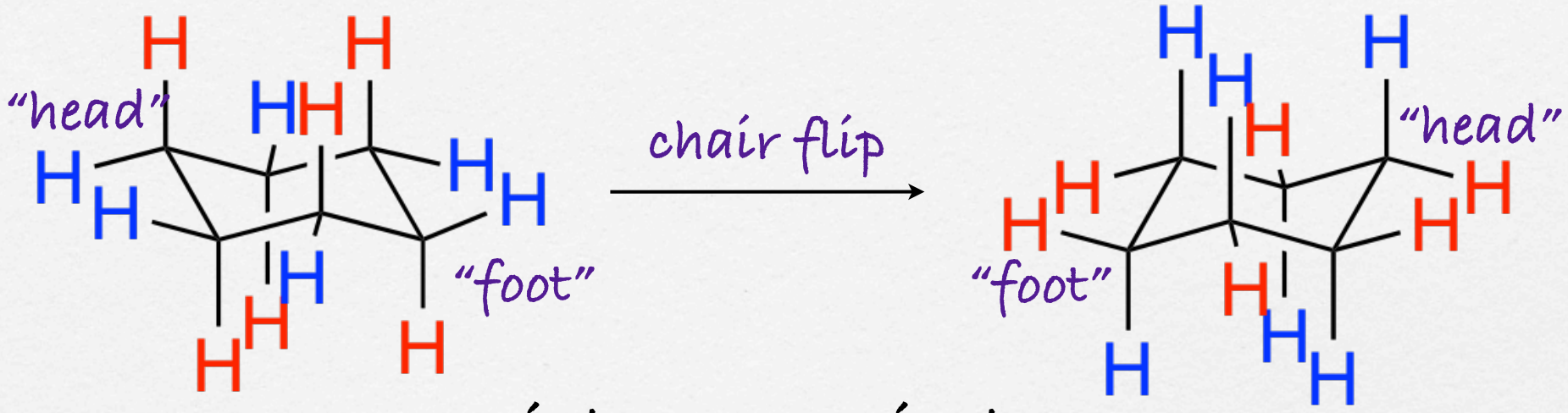


boat





A Closer Look at Chair Conformers



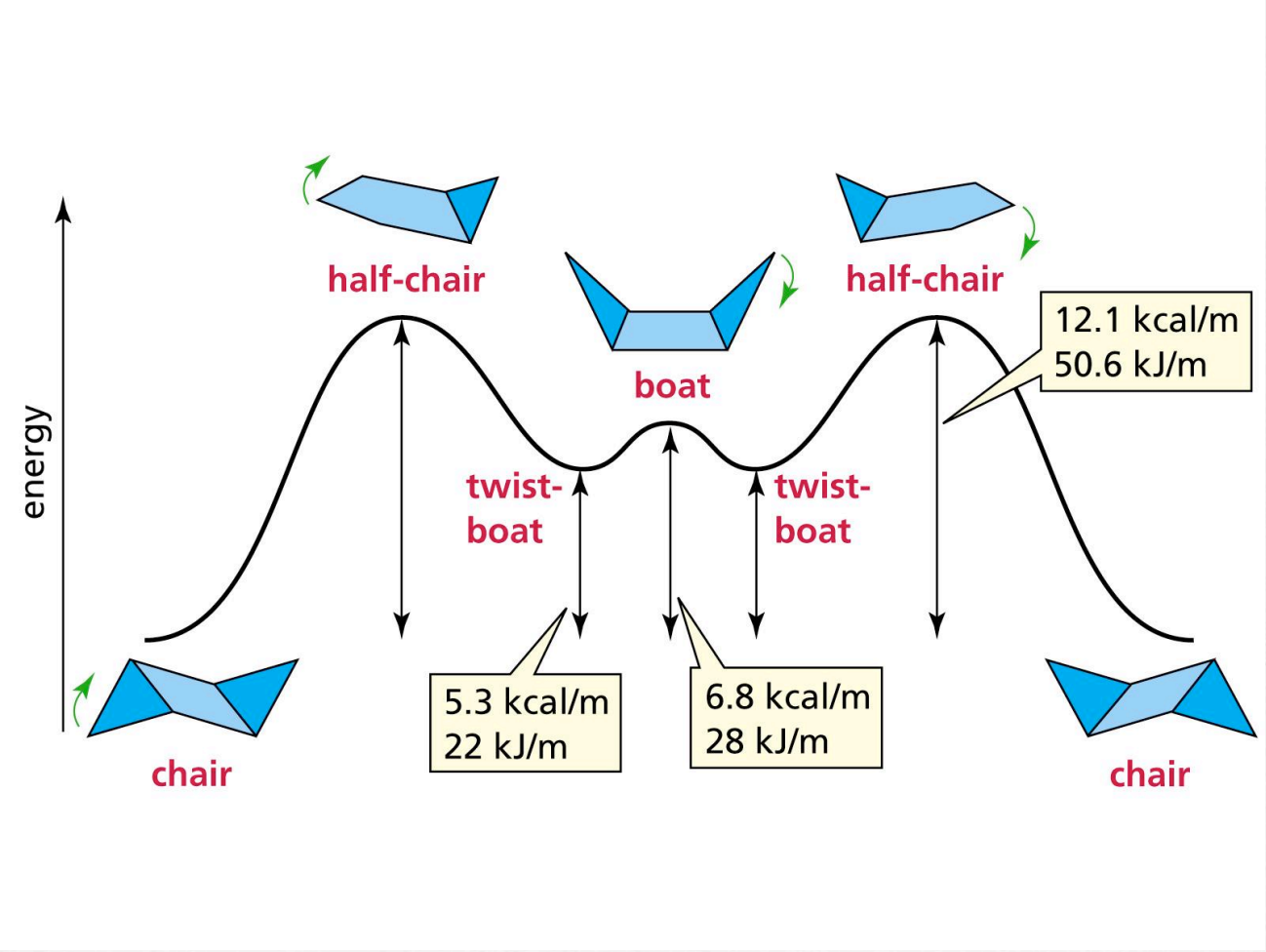
axial H = vertical H

equatorial H = horizontal H

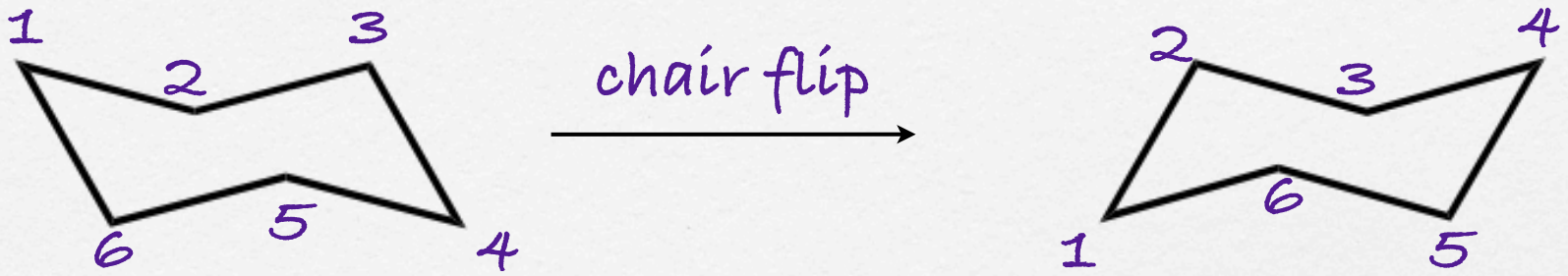
Each C has 1 axial H & 1 equatorial H

Chair Flips: The Molecular Process

barrier to chair flip = 10-12 kcal/mol



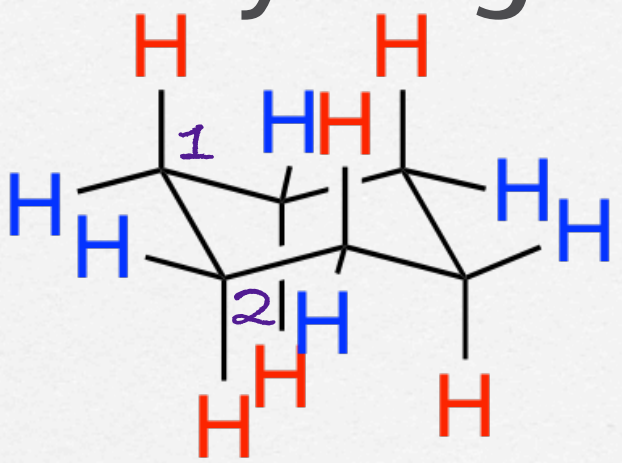
Drawing Chair Flips: Carbons



1. Number carbons
2. Draw flipped chair
3. "Head" becomes "foot".
4. Number appropriately.

DON'T CHANGE ORDER!!!

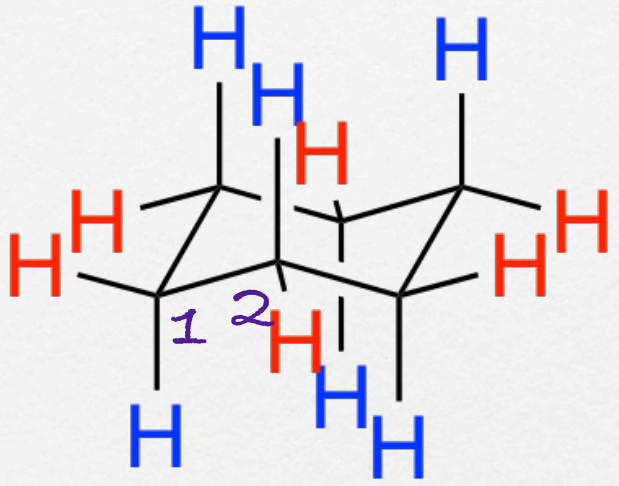
Drawing Chair Flips: Hydrogens



axial

equatorial

chair flip

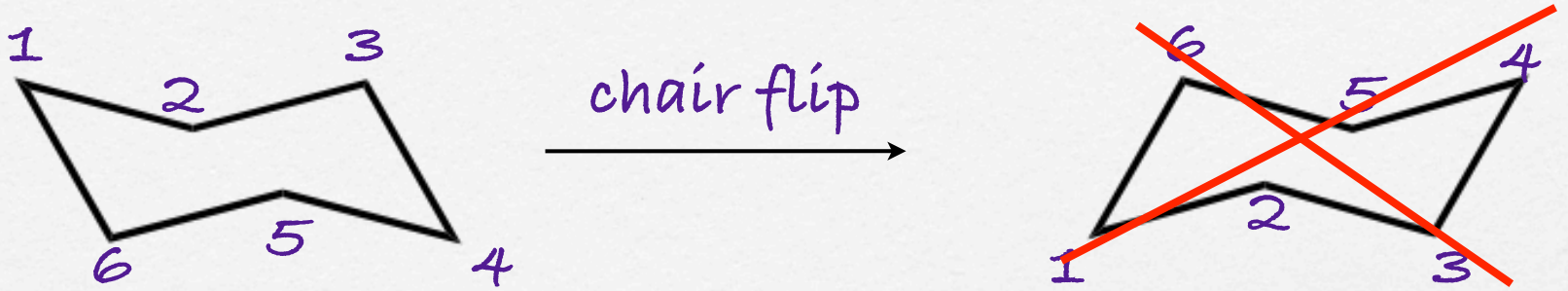


axial

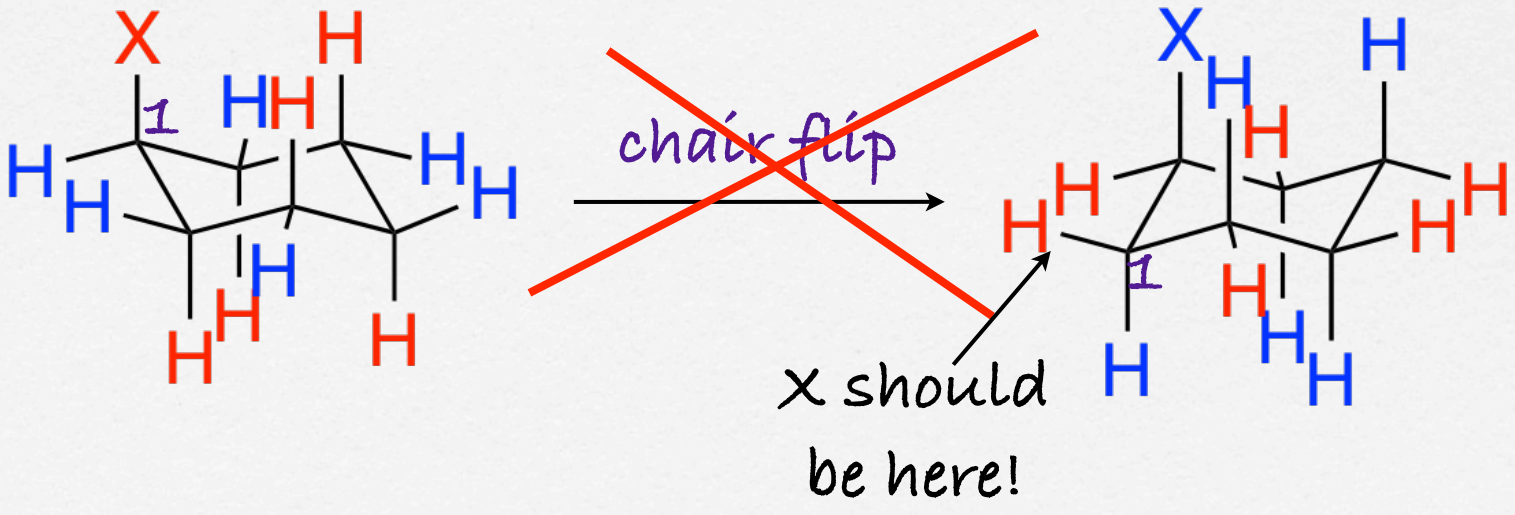
equatorial

After flip, axial becomes equatorial & equatorial becomes axial.
Up stays up! Down stays down!

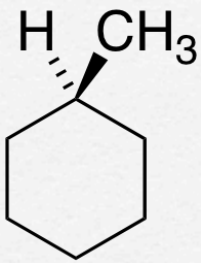
Common Chair Flip Mistakes

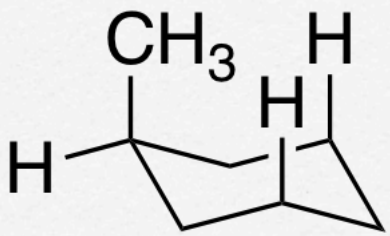


Don't change direction of #s!

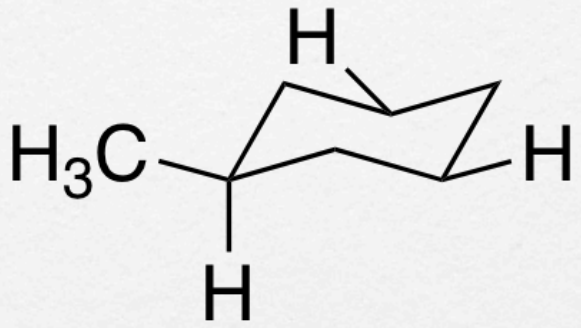


Monosubstituted Chairs

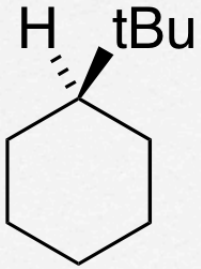


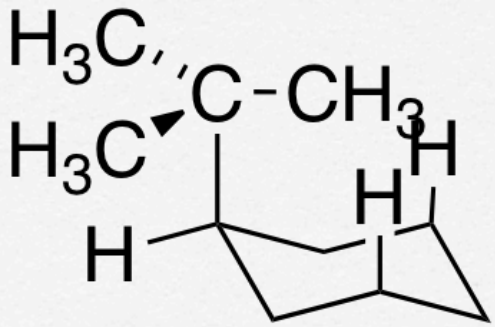


1.8 kcal/mol

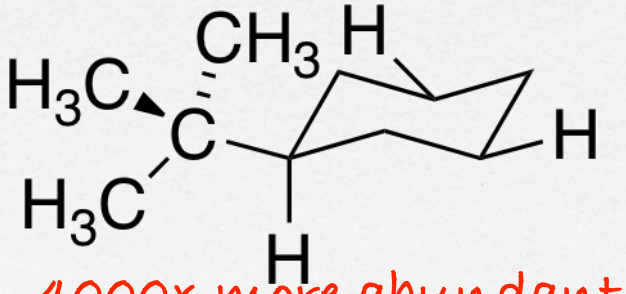


~20x more abundant





5 kcal/mol

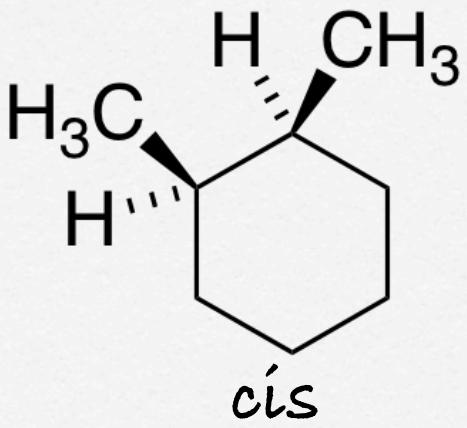


4000x more abundant!

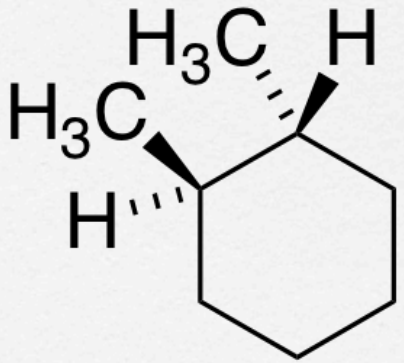
A Note on Stereoisomers

- Stereoisomers: differ by spatial arrangement
- Cis: same side
- Trans: opposite side

stereoisomers

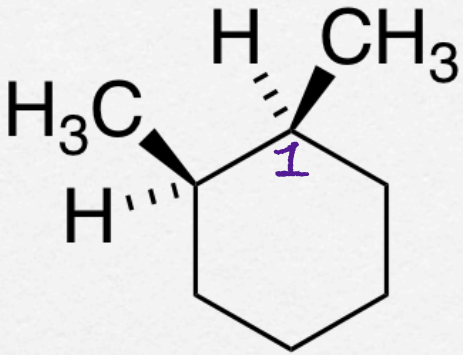


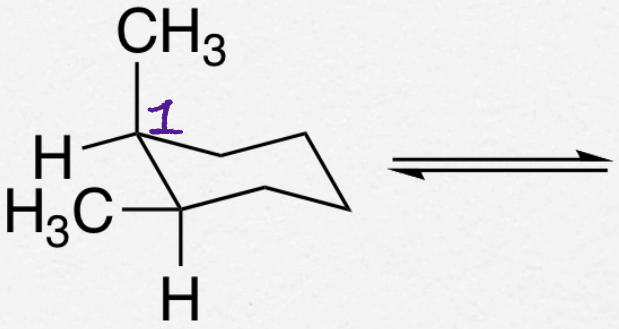
cis

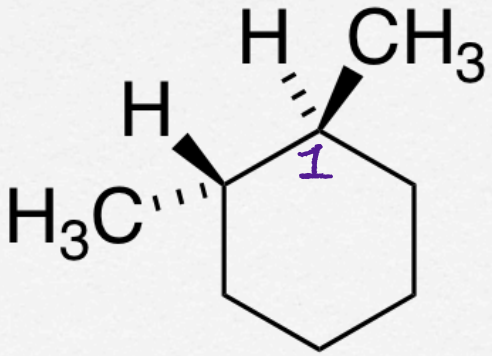


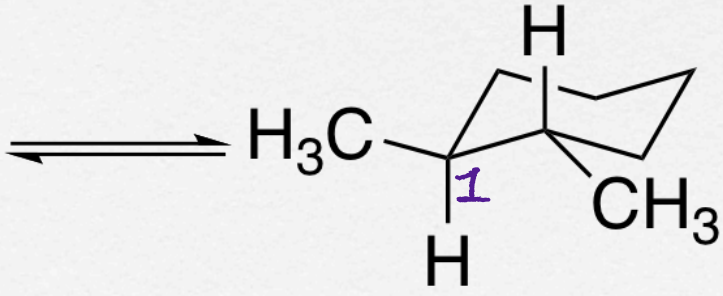
trans

Disubstituted Chairs: 1,2

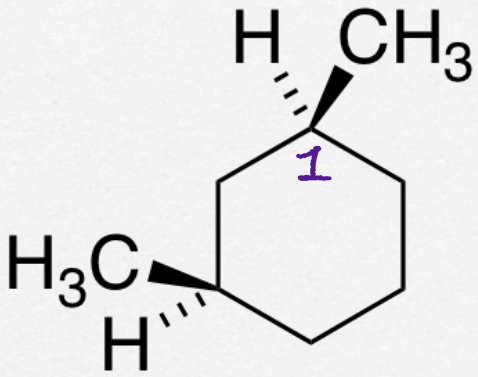


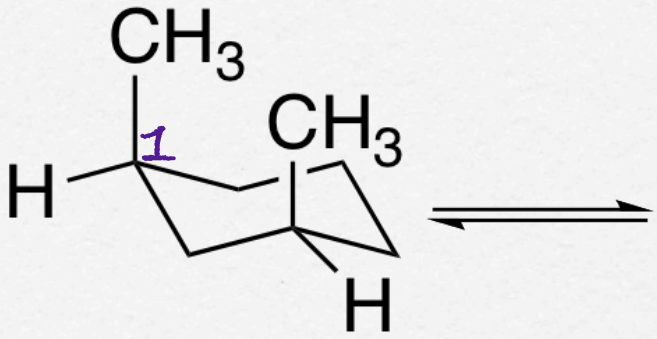


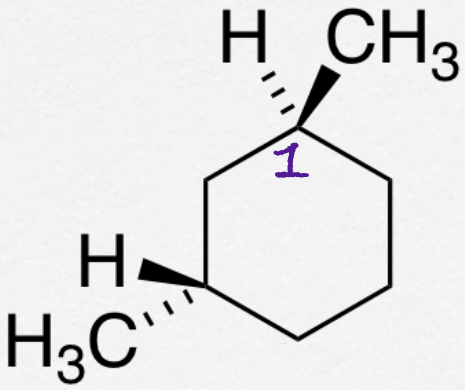


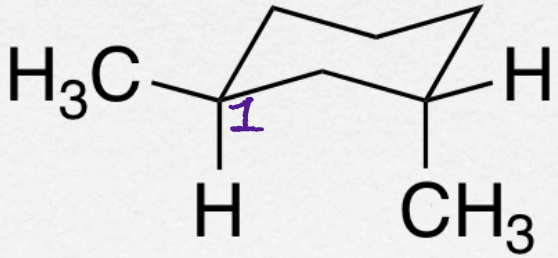


Disubstituted Chairs: 1,3

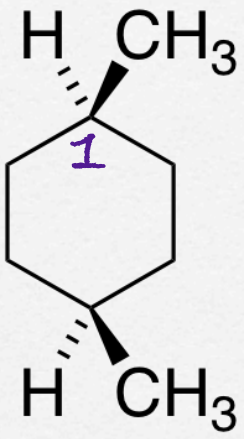


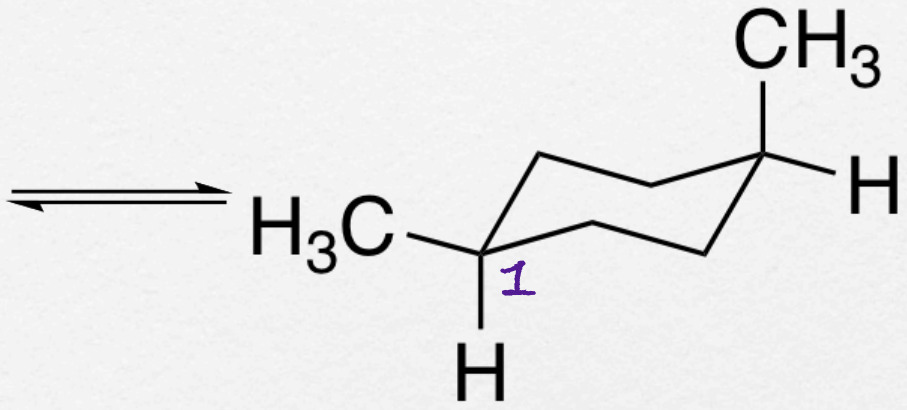


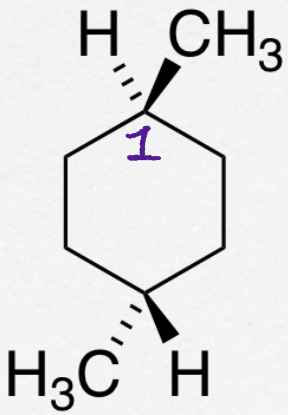


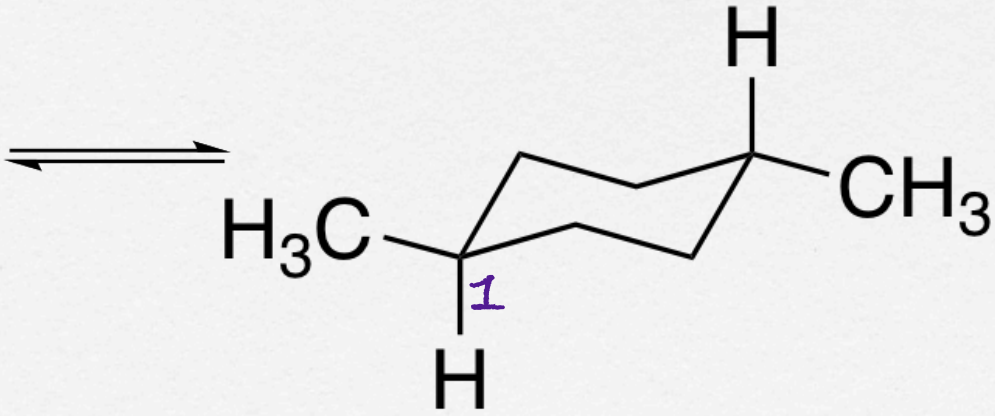


Disubstituted Chairs: 1,4









Chair Conformers Energy Summary

- Having groups in axial positions is generally higher energy than having them in equatorial positions
- A t-Bu group will not be in an axial position
- When something MUST be axial, having smaller groups axial will be lower energy

Wrapping Up

- Practice drawing both chair conformers
- Practice drawing in axial and equatorial positions on each carbon of the chair
- Practice identifying cis and trans isomers
- Practice chair flips with substituents
- Practice identifying the lower energy conformer