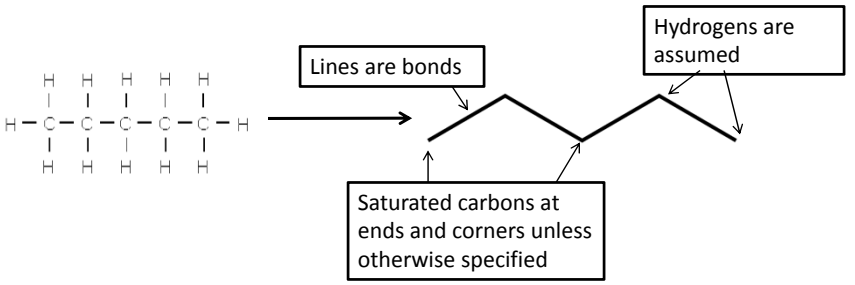
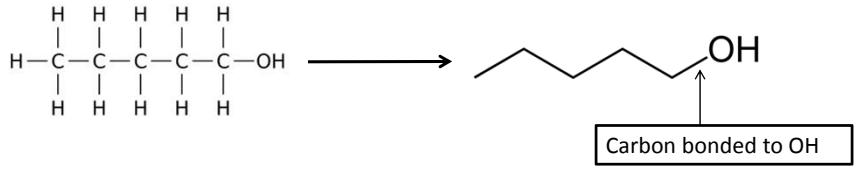
Stereochemistry

May 7, 2012

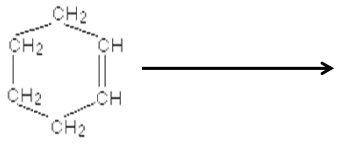
UC Davis GAANN Fellowship

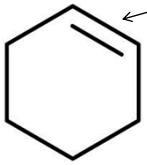
Review 2-D Drawings





Review 2-D Drawings

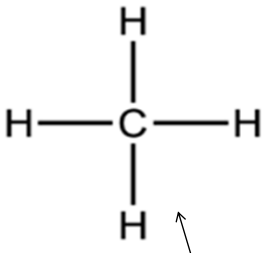


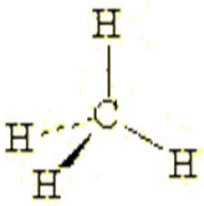


Double bond represented by 2 lines

3-D Drawings

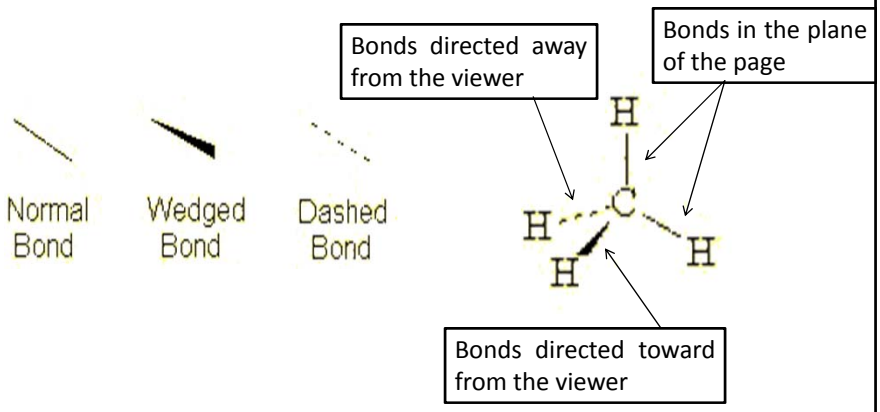
3-D drawings more accurately represent bond angles, molecular shape, and differentiation of isomers



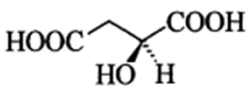


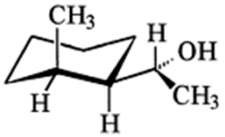
Does not illustrate shape or bond angles

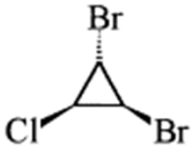
3-D Drawings: Bonds

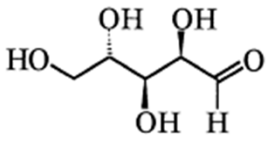


3-D Drawings: More examples



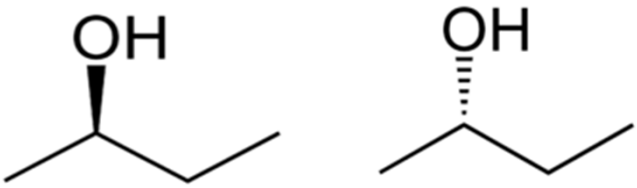






Stereochemistry

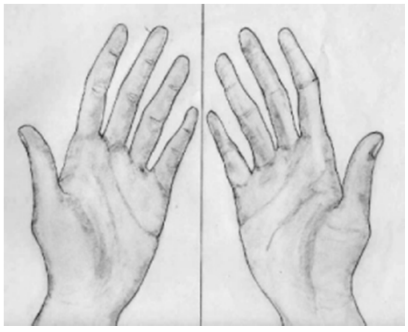
Stereochemistry is the study of spatial properties of molecules that have the same formula and connectivity but have different 3-D shapes



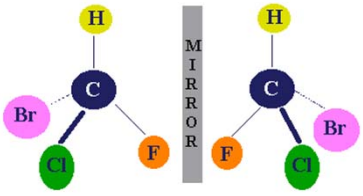
Stereoisomers are molecules with identically connected atoms but oriented differently in space

Chiral Molecules

Entantiomers are stereoisomers which are mirror images of each other



http://www.ilc.uni-hohenheim.de

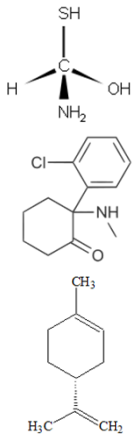


http://web.fccj.org

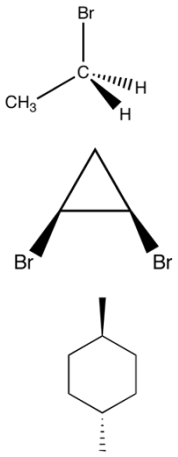
Chiral molecules are nonsuperimposable stereoisomers on their mirror. (ie, they show "handedness".)

Examples of Chirality

Chiral Molecules

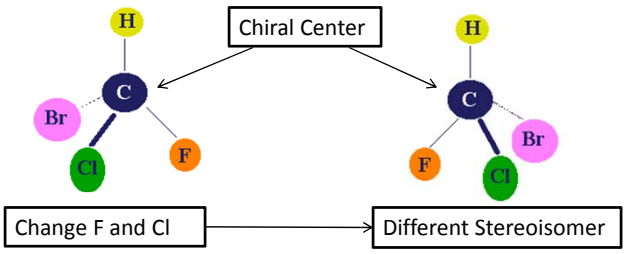


Achiral Molecules



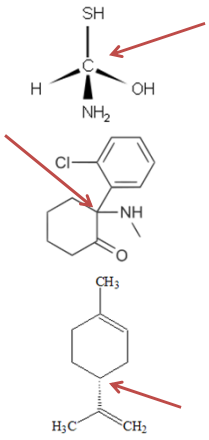
Chiral Centers

Chiral centers are atoms, where the interchanging of any two bonds will result in the formation of a different stereoisomer.

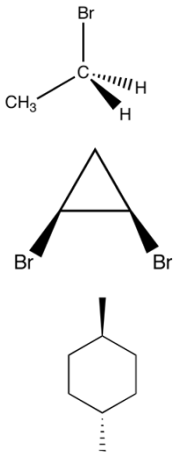


Chiral Centers

Chiral Molecules

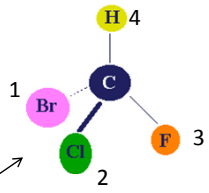


Achiral Molecules



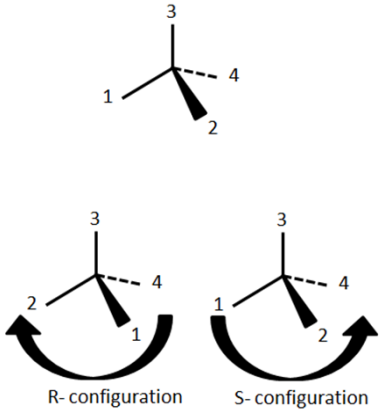
Chiral Center Configuration

- Each chiral center has 2 possible configurations: R or S
- Rules for determining configuration:
  1. Assign each substituent a priority from 1 to 4 based on the following rules:
     - A. Higher atomic number = higher priority
       I > Br > Cl > F > O > N > C > H
     - B. If two atoms have the same atomic number, priority is determined by the "secondary" substituents
     - C. If there are double or triple bonds on the secondary substituents, they are treated as 2 or 3 bonds.



Chiral Center Configuration

2. Orient the center such that priority number 4 is directed into the page
3. Determine R or S configuration by the direction of decreasing priority (increasing number)
   - Priority increases clockwise- R configuration
   - Priority increases counter-clockwise, S configuration

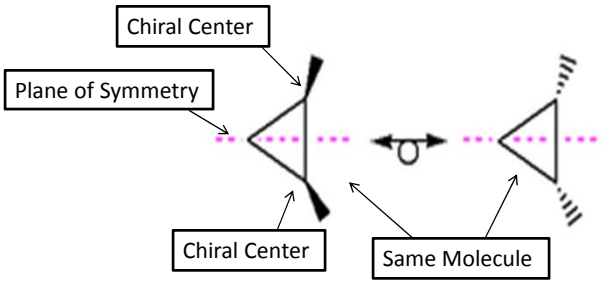


Example of Chiral Center Configuration Determination

Multiple Chiral Centers

If a molecule has multiple chiral centers, this **does not** mean its chiral.

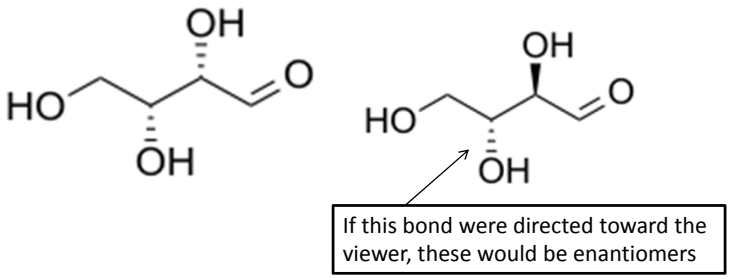
Any molecule with a plane of symmetry is achiral.



Diastereomers

Diastereomers are pairs of molecules with more than one chiral center that are not mirror images of each other.

These molecules would be considered enantiomers if all chiral centers were opposite.



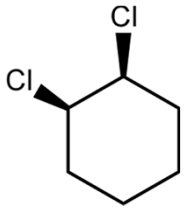
Examples of Diastereomers

Conformational Isomers

- Double bonds result in rigid structure, preventing bonds from changing conformation.
- If both carbons contain two substituents, two formations are possible:
  - Cis- “same side”
  - Trans- “opposite side” – add pictures

Comformation Isomers

Cis



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