Lab Activity #1: Molecular Models

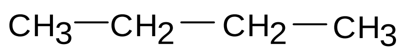
<u>Objectives:</u>

1. To make 3-dimensional models of various molecular and organic chemicals
2. To understand the molecular geometry with respects of VSEPR and molecular models
3. To study Geometric (Constitutional) Isomers, Stereo-Isomers, Conformational Analysis using Newman Projections, and Chiral Enantiomers.

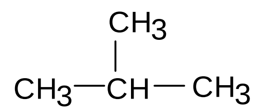
<u>Background Information:</u>

1. <u>Geometric (Constitutional) Isomers</u>: - compounds that have the same chemical formula but different structural formulas.

Example: C_4H_{10} has two geometric isomers.



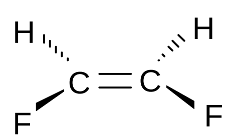
butane



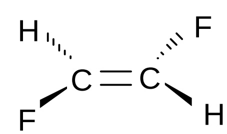
methylpropane

2. <u>Stereo-Isomers</u>: - compounds that have substituents on the same side (*cis*-) or opposite sides (*trans*-) across the double bonds.

Example: 1,2-dicfluoroethene has two stereo-isomers.



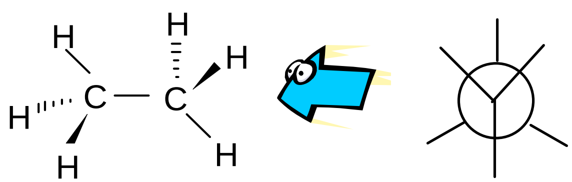
cis-1,2-difluoroethene



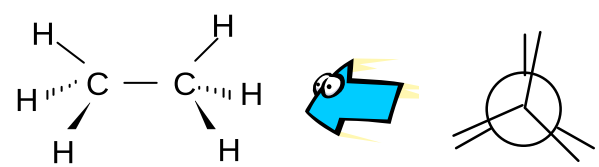
trans-1,2-difluoroethene

3. <u>Conformational Analysis</u>: - compounds when containing single bonds can rotate between two centers. A certain conformation is preferred at different temperature due to the energy required to achieve such conformation. These conformations can be shown easily using a **<u>Newman Projection</u>** when the molecule is view when the two centers are overlap along a line of sight.

Example: There are two conformation of ethane.

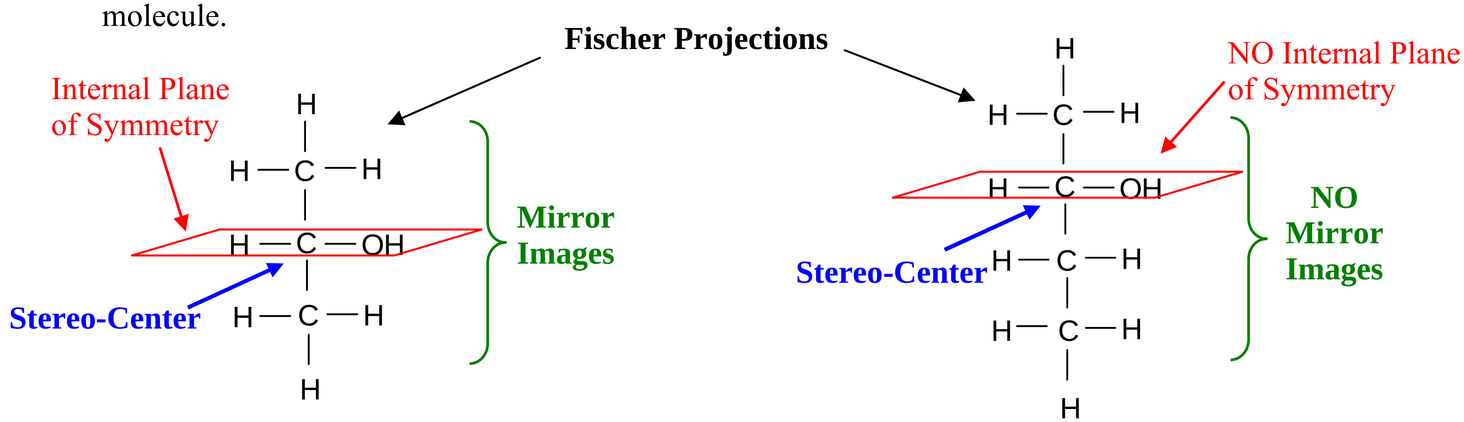


***Staggered Conformation* and the Newman projection**
(Lower Energy – least crowded; favor in low temperature)



***Eclipsed Conformation* and the Newman projection**
(Higher Energy – more crowded; favor in high temperature)

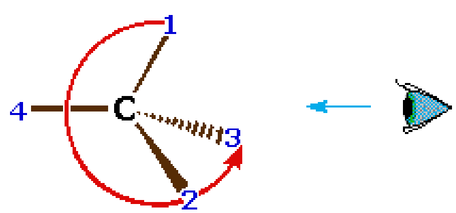
4. <u>Chiral Enantiomers</u>: - are non-super-imposable mirror images of one another. Not being able to superimpose one molecule on top of the other simply means that the two molecules are not equivalent or identical. For a compound to form an enantiomeric pair, it must have **<u>chiral molecules</u>**. **<u>Chiral molecules must not have an internal plane of symmetry, and they must have a stereo-center</u>.** We can use **<u>Fischer Projection</u>** (as view from above) to analyze the chirality of a molecule.



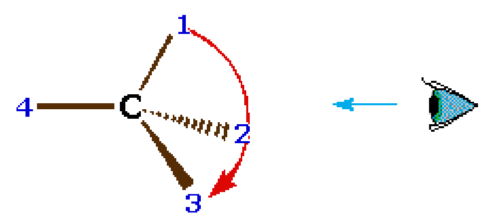
<u>Achiral Molecule</u>: - an internal plane of symmetry about the stereo-center reveals mirror images.

<u>Chiral Molecule</u>: - there is no internal plane of symmetry about the stereo-center (no mirror images).

<u>Enantiomeric Conformations</u>: - there are always two enantiomers for a chiral compound. They are **<u>(*R*) conformation</u>** ("rectus" – Latin for **<u>right</u>**) and **<u>(*S*) conformation</u>** ("sinister" – Latin for **<u>left</u>**).
- the direction for **<u>left (counter-clockwise)</u>** and **<u>right (clockwise)</u>** is determined after the substituents of a chiral molecule is assigned priority (1 is the highest priority and 4 is the lowest).



(*S*)



(*R*)

The Sequence Rule for Assignment of Configurations to Stereogenic (Stereocenter) Carbons

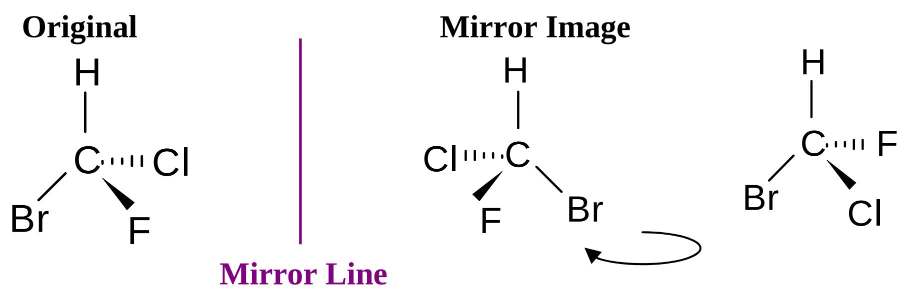
Assign sequence priorities to the four substituents by looking at the atoms attached directly to the chiral stereogenic carbon atom.

1. The higher the atomic number of the immediate substituent atom, the higher the priority.
   For example, H– < C– < N– < O– < Cl–. (Different isotopes of the same element are assigned a priority according to their atomic mass.)

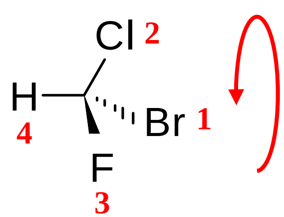
2. If two substituents have the same immediate substituent atom, evaluate atoms progressively further away from the chiral center until a difference is found. For example, CH_3– < C_2H_5– < $ClCH_2$– < $BrCH_2$– < CH_2O–

3. If double or triple bonded groups are encountered as substituents, they are treated as an equivalent set of single-bonded atoms.
   For example, C_2H_5– < CH_2=CH– < HC≡C–

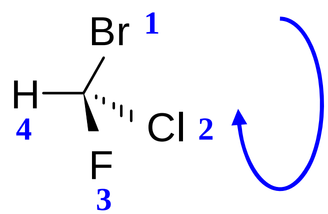
Example: There are two enantiomers for CHBrFCl.



Note that by rotating the bottom (so that H remains up and Br is to the left), we cannot make the mirror image equivalent to the original (non-super imposable).



(*S*) bromochlorofluoromethane



(*R*) bromochlorofluoromethane

Materials:

Organic Molecular Model Kit

Procedure:

1. Copy the following table in your lab notebook (landscape orientation would be the best).
2. Fill in the table. If the compound has stereo-isomers, for example, draw and name the structure. The same apply enantiomers. If the cell does not apply, write N/A.

Name	**Class of Molecule**	**Functional Group**	**Structural Formula (3-D)**	**Stereo-isomers (cis or trans)**	**Conformational Analysis (Newman Projection)**	**Chiral or Achiral (Show Plane of Symmetry and Stereocenter)**	**Enantiomers**
Methane	*alkane*	*R*					
Ethane							
Propane							
1-iodopropene							
3-chloropropyne							
Cyclopropane							
Cyclobutane							
Cyclopentane							
Cyclohexane							
1,2-difluorocyclohexane	*haloalkane*	*R−X*					
chlorofluoromethanol							
Ethanol							
Ethylmethyl ether							
2-butanone							
Propanal							
ethanoic acid							
propyl methanoate							
Methylethylamine							
Benzene							
p-difluorobenzene							