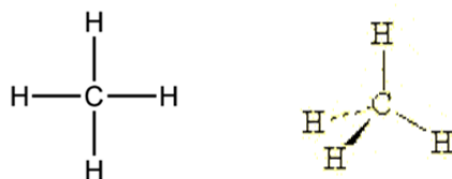


Prelab Reading and Questions

Review 3-D Drawings

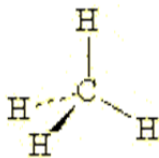
Organic molecules are generally three dimensional structures, so it is more accurate to represent them with three dimensional drawings. The benefit of using three dimensional drawings is the inclusion of bond angles, the molecules shape, and differentiation of isomers. In 2-D drawings, bonds are often represented as lines for simplicity and speed. Three dimensional sketches can be done in a similar manner, with some alterations to represent bonds in different planes.



A fully saturated carbon molecule has a tetrahedral shape, with 4 different bonds. If two of these bonds are in the same plane as the page it is drawn on, one bond will be directed into the page and another will be directed out of the page. Bonds in the same plane as the page are simply represented as a solid line. Bonds directed into the page are represented by a dashed line. Bonds directed out of the page are represented by a “wedged” line.



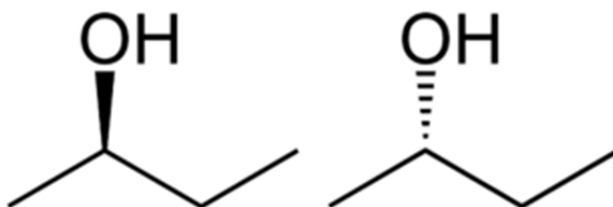
These bonds can be used to accurately represent a tetrahedral molecule, such as the following methane molecule:



This method can also be used for more complex molecules. Again, all bonds in the plane of the page are represented by normal lines. Bonds pointed towards the viewer are represented by wedges. Bonds pointed away from the viewer are represented by dashed lines. It is helpful to make the main backbone of the molecule in the plane of the page, with other substituents directed into or out of the page.

Stereochemistry

In this lab we will study, **stereochemistry**, which is the study of the spatial properties of molecules that have the same formula and connectivity but have different 3-D shapes. This is particularly relevant in organic chemistry due to the structure of carbon bonding and larger size of molecules which give rise to different possible 3-D structures. The 3-D structure contributes to the functionality and activity of molecules which is extremely important for certain applications. For example, certain pharmaceutical chemicals can be lethal if the 3-D structure is not perfect. A simple example of stereochemistry is exhibited by 2-butanol.



As can be seen from the 3-D drawing above, the molecule has 2 possible 3-D structures for the same formula and bonding connectivity. These are called **stereoisomers**, which are defined as molecules with atoms identically connected, but oriented differently in space. These

molecules are also mirror images of each other. When 2 stereoisomers are mirror images of each other, they are considered **enantiomers**, which is a subclass of stereoisomers.

Chiral Molecules

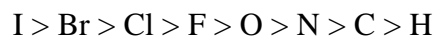
Some molecules that exhibit stereoisomerism are called **chiral** molecules. Chiral molecules are non-super imposable on their mirror image which means that these molecules have handedness. An obvious example of handedness is your hands. Clearly, your hands are not identical and cannot be superimposed by reorienting them, but they are mirror images of each other. This is true of the 2-butanol example as well. The chirality of a molecule and also be determined base on the presence of a plane of symmetry. If a molecule has a plan of symmetry, it is **achiral** (not chiral). It is important to realize that a plane of symmetry can be found in any dimension, thus a 2-D molecule will always be achiral because there is plane of symmetry in the molecular plane.

As was mentioned above, the bonding structure of carbon plays a key role in determining the 3-D structure of organic molecules. In particular, a tetrahedral carbon (carbon with 4 single bonds) with all different substituents is always chiral because if these substituents are reoriented a stereoisomer is formed. Such carbons are considered **chiral center**, which is defined as an atom for which an interchanging of any 2 ligands forms a stereoisomer. In the case of the 2-butanol shown above, the second carbon is the chiral center with -OH , -CH_3 , $\text{-CH}_2\text{CH}_3$, and -H as the 4 different substituents.

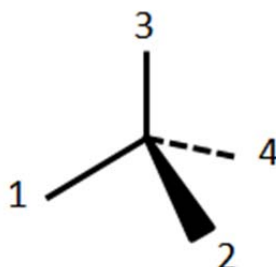
Chiral Center Configuration

Each chiral center has 2 possible configurations which are classified as R or S. This classification is determined based on the arrangement of the substituents attached to the carbon using the following procedure.

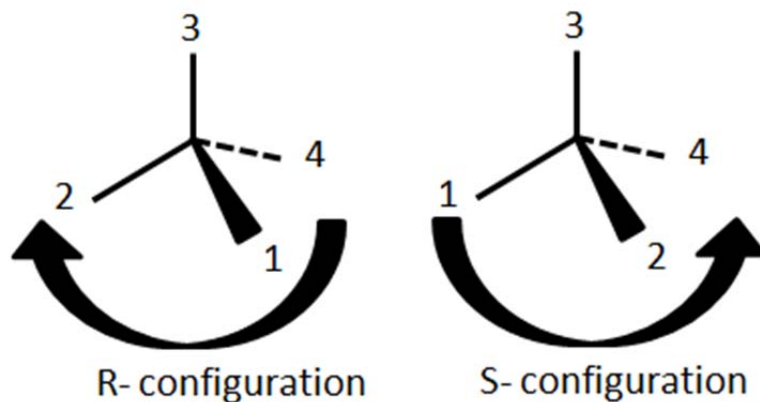
1. The substituents attached to the carbon atom are assigned numbers from 1 to 4 based on priority level shown in the scales below and the listed rules (#1 is highest priority)



- The higher the atomic number the higher the priority.
 - If 2 of the substituents have the same priority based on the attached atom, the priority is based on that atom's substituents.
 - If there is a double or triple bond attached to the substituent, it is treated as though it has 2 or 3 single bonds respectively, which are bonded atoms as is shown schematically in
2. The center is oriented such that substituent number 4 is pointing into the page as shown.



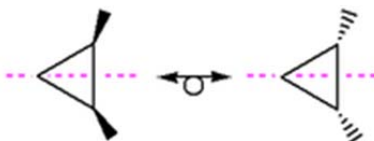
3. R- and S- configuration are determined by direction of decreasing priority. Starting at 1, if the priority number increases in a clockwise fashion, the chiral center is considered to have an R- configuration. If the priority number increases in a counter-clockwise fashion, the chiral center is considered to have an S-configuration.



The R and S configurations can be used to classify stereoisomers as well. If a molecule only has 1 chiral center, then the R and S molecules are enantiomers.

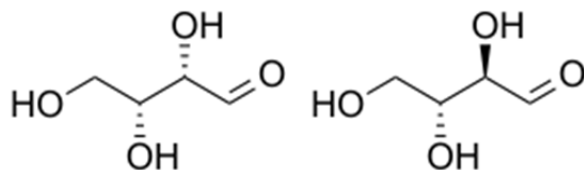
Multiple Chiral Centers

Molecules with multiple chiral centers are a bit more complicated. The presence of these chiral centers does not necessarily indicate that the molecule is chiral because the chiral centers can be distributed within the molecule in a symmetric fashion. As stated above, any molecule with a plane of symmetry is achiral. Molecules that exhibit a plane of symmetry but contain multiple chiral centers are called meso compounds. An example of this is 1,2 methyl substituted cyclopropane shown below. Despite the presence of 2 chiral centers, the molecule is symmetric and thus achiral.



Enantiomers can also be identified based on R and S configuration of the different chiral centers for molecules with multiple chiral centers. If 2 stereoisomers have opposite configuration (R vs. S) for every chiral center in the molecule, then they are enantiomers. If some of the chiral centers are opposite configuration, but not all of them are, the molecules are

diastereomers. Diastereomers is another subclass of stereoisomers. These are stereoisomers that are not enantiomers, and thus not mirror images of each other. An example of this is threose and erythrose which is shown below. In this figure only 1 of the 2 chiral centers is switched, leading to a diastereomer. If the other chiral centers were switched, the result would a pair of enantiomers.

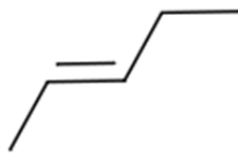


Conformational Isomers

Another type of stereoisomer is conformational isomers. Conformational isomers consist of the different molecular structures formed from rotating a bond. These are generally ignored for single bonds because at ambient temperatures the bonds are always rotating. However, double bonds are rigid, and do not rotate unless they undergo reaction. If both carbons participating in a double bond have 2 different substituents, then the molecules can take on 2 orientations called cis and trans. If each respective substituent of highest priority (according to the priority rules above) on either side of the double bond are on opposite sides of the molecule, then the molecule is trans. If they are on the same side, the molecule is considered cis. This can be seen in 2-pentene as shown below. In this molecule, the highest priority on the left side is the methyl group, while the highest priority on the right side is the ethyl group. When these are oriented above and below the molecule, they are trans, and when they both oriented above or both oriented below the molecule, they are cis.



cis-2-pentene



trans-2-pentene