Molecular Models/ChemDraw®

Your first experiment of the fall semester is devoted to building models of organic compounds with the Darling Framework Molecular Models kit that came with your CHM 241 textbook, and with the chemical drawing program ChemDraw®. Learning how to envision organic compounds with the use of models will be critical to your understanding of many important topics in organic chemistry. We will examine two of those topics in Expt #1: constitutional isomers and *cis-trans* isomers.

The chemistry of organic compounds is to a large extent controlled by their 3-dimensional structures. These structures, in turn, are a function of the bonding patterns of carbon atoms:

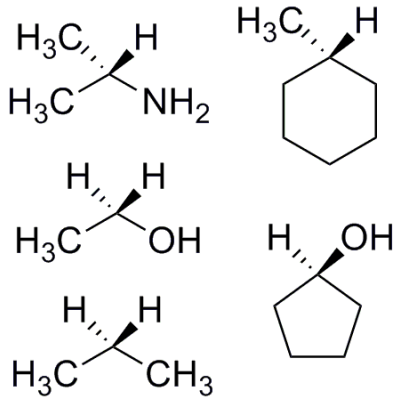
• carbon atoms form strong bonds to other carbon atoms that lead to molecules with large carbon frameworks

•carbon atoms form strong covalent bonds to most other elements leading to a wide variety of structural and functional variation

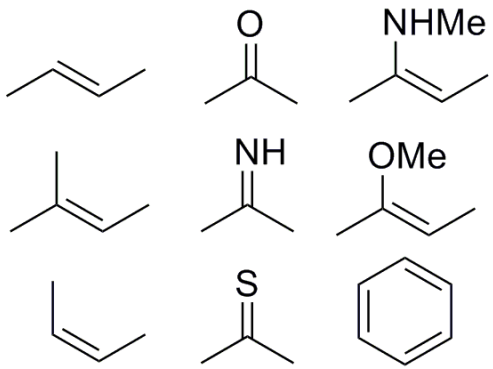
•carbon atoms can bond to 2, 3, or 4 other atoms leading to a wide variety of molecular shapes

Molecular Shapes

The variety of molecular shapes is a function of the fact that carbon bonds to 4 other atoms (sp^3 carbon) to form a tetrahedral structure with bond angles of ca. 109.5°, 3 other atoms (sp^2 carbon) to form trigonal planar structures with bond angles of ca. 120°, and 2 other atoms (sp carbon) to form linear structures with 180° bond angles. Examples of these structures are shown below. Remember that H atoms are usually not represented in these bond-line drawings unless needed to clarify a structure or to emphasize a point, or if bonded to a heteroatom.



tetrahedral (sp^3) carbon

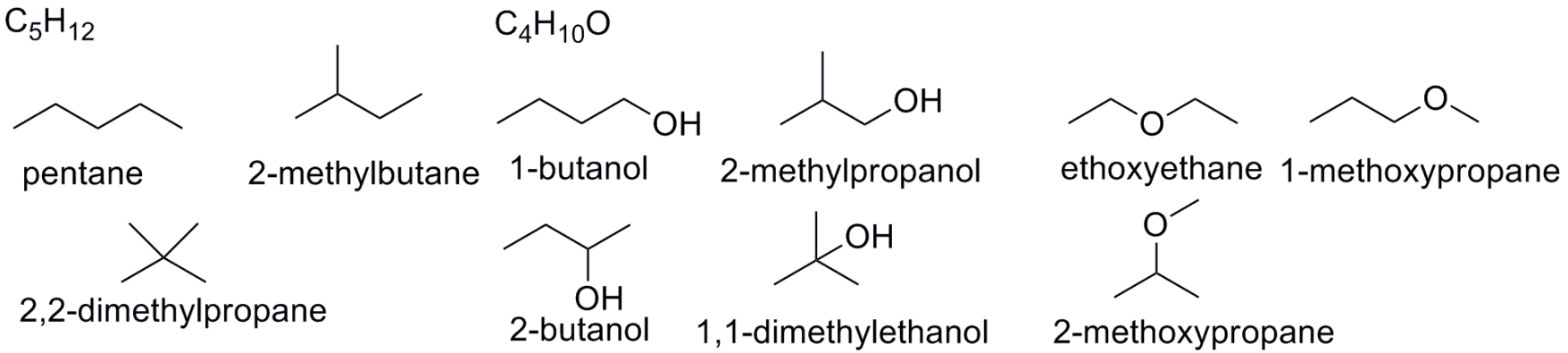


trigonal (sp^2) carbon

linear (sp) carbon

Constitutional isomers

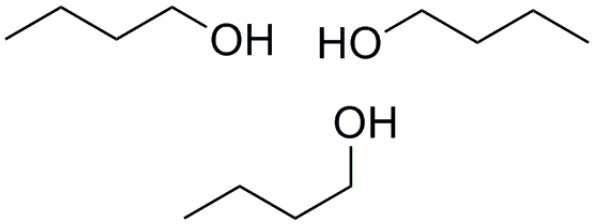
Constitutional isomers (isomers with different bond connectivity) arise in organic compounds as a result of differing carbon-carbon bond frameworks, differing placement of functional groups, and different functional groups. Examples of all three cases are shown below.



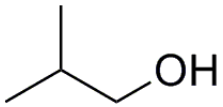
The three constitutional isomers of C_5H_{12} exist because of differing C-C bond connectivity patterns. The seven constitutional isomers of $C_4H_{10}O$ exist because of different C-C bond connectivity, differing placement of the functional groups, and the fact that the formula is consistent with two different functional groups: alcohols and ethers.

Constitutional isomers or equivalent structures?

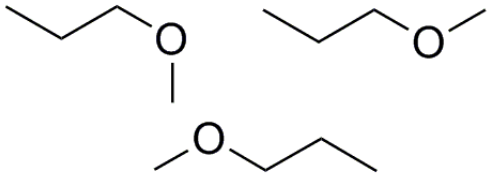
Beginning students often have trouble distinguishing different ways to draw the same compound (equivalent structures) from constitutional isomers. This experiment will help you to address this issue with the help of molecular models. Naming the compounds often helps



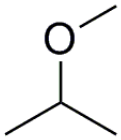
equivalent structures of
1-butanol



constitutional isomer
2-methylpropanol



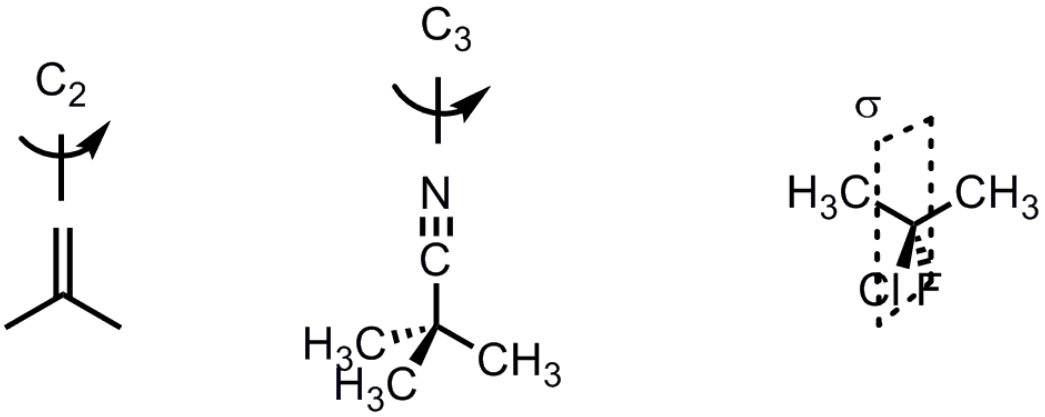
equivalent structures of
1-methoxypropane



constitutional isomer
2-methoxypropane

Equivalent atoms within the same structure

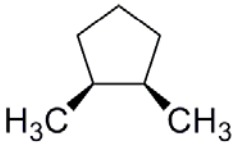
It will be important for you to recognize equivalent atoms within a structure to understand chemical reactivity and the spectroscopic properties of compounds. Equivalent atoms are atoms that can be superimposed on each other by rotation about a rotational axis that exists in the molecule or by reflection through a mirror plane that exists in the molecule. Examples are shown below.



In this experiment you will explore the concept of equivalent atoms with the help of ^{13}C NMR spectra of various compounds. ^{13}C NMR spectra have the property that equivalent carbon atoms give overlapping signals, so the number of ^{13}C signals seen in the ^{13}C NMR spectrum of a compound counts the number of unique carbon atoms in the molecule.

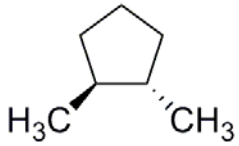
Cis-trans isomers

In this experiment you will also explore *cis-trans* isomers which exist because of hindered rotation around a single bond in a ring structure or about a double bond. These are examples of a new kind of isomer: stereoisomers. Stereoisomers have the same bond connectivity, but differ in the 3-dimensional arrangement of atoms in space. *Cis-trans* isomers are examples of a type of stereoisomer called diastereomers. You will learn more about these and another type of stereoisomer, enantiomers, in a few weeks in CHM 241.



cis-1,2-dimethylcyclopentane

cis-2-butene



trans-1,2-dimethylcyclopentane

trans-2-butene

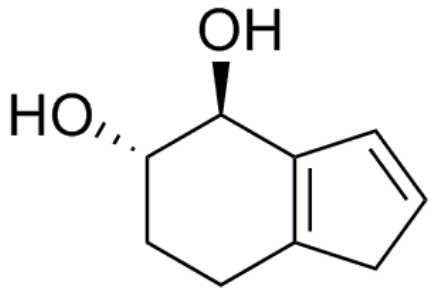
The *cis*- prefix means “on the same side”, while *trans*- means “opposite” or “across from”.

Learning to use ChemDraw®

You will learn to use this drawing program largely by using it, but the following exercise can get you started.

An exercise in using ChemDraw

Suppose this is your target:



Open the program
1. Click on "File" in the main toolbar
2. select "New Document"
3. select "Apply document settings from"
4. select "ACS Document 1996"

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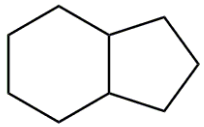
Setting up the carbon backbone



5. set the scale to 200%
6. select the "cyclohexane ring" tool in the drawing tool box
7. click in the drawing area to insert the ring
8. select the "cyclopentane ring" tool
9, put the cursor on a bond of the cyclohexane ring at about the midway point of the bond and click

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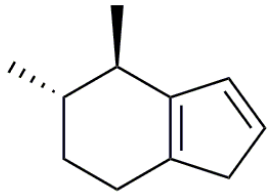
Inserting wedged and hashed bonds and multiple bonds



10. select the solid "wedged bond" and click on the cyclohexane ring at the indicated carbon
11. select the "hashed wedged" bond from the drawing tool bar
12. click on the indicated carbon and the bond will be placed where you want it to go
13. select the "solid bond' tool
14. place the double bonds where you want them by clicking in the middle of the single bonds

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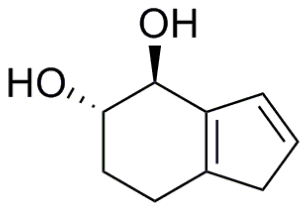
Inserting heteroatoms



15. select the "text" tool, click on the end of the wedged bond and type "OH"
16. go to the other wedged bond and insert the "OH"
17. you can also accomplish heteroatom insertion by selecting the lasso tool instead
18. click on the end of the bond, and type "o", "OH will appear
19. do the same thing for the other hydroxyl group
20. the second method requires fewer key strokes, but sometimes the program misunderstands

Keep Practicing!! Don't forget to save files when you get the drawings in the final form. You can also save the files as tiff files that are easily imported into Word documents via the "insert picture" command. The tiff files cannot be re-opened by ChemDraw®, so make sure you always save the original (cdx) file.

This Week's Experiment.

This is a two part experiment:

- **Part 1: You will use the Darling Framework Molecular Models to complete several exercises that explore equivalent structures, equivalent atoms within structures, constitutional isomers, and *cis-trans* isomers. Your particular assignment will be given to you at lab time. Do not forget to bring the model kit with you!!**
- **Part 2: The exercises for this part are already written up in the Manual. These exercises explore constitutional isomers and *cis-trans* isomers in the context of the chemical drawing program ChemDraw®. Download the program to your laptop before coming to lab using the directions posted on Niihka. Bring your laptop to lab!!**