Laboratory 7: Organic Molecule Models

(This lab was developed by Laura Sonnichsen and modified by Laura Sonnichsen and Virginia Lehmann.)

References:

Merlic, J. Chemistry 11 Lab Manual (1998) New York: Harcourt Brace.

Timberlake, K. C. Essential Lab Manual to accompany Chemistry: An Introduction to General, Organic, and Biological Chemistry, 8^{th} ed. (2003) New York: Benjamin Cummings

Report Requirement: Answer all of the questions/do all the computations requested in *italics*. Questions not in italics do NOT need to be answered. You do NOT have to write a formal lab report. You should write your answers into a word processing program and save the file either as a Rich Text Format (.rtf) or html file. Go into the Lab #7 Report and cut and paste the answers to each question in the appropriate space. (Lab #7 Report can be found on the Content page or under Assignments → Quizzes.)

There are also drop boxes for questions 2, 4 and 6. Either type your structures and save each question answer as a separate .html, .rtf or .pdf file OR neatly hand-draw the structures and scan to three separate .pdf files. (Lab #7 Question 2 drop box, Lab #7 Question 4 drop box and Lab #7 Question 6 drop box are under Assignments → Dropbox)

Labs not submitted in the appropriate area will *not* be graded.

Report Scoring: 20 points total (each part). Questions valued as marked.

Working with a Partner: You are permitted to work with a partner. If you do so, the experimental data reported may be the same, but you need to write your own answers to each question. At the beginning of each question you should note that you worked with a partner by writing "Lab Partner (fill in name)."

Materials:

- Model kit (found in CHE 106 Lab Kit)
- A protractor (to measure angles)

Goals:

1. To help you visualize the 3-D structure of organic molecules.
2. To teach you how to use model kits
3. To learn how to differentiate among the three types of isomers (structural, geometric, and stereoisomers)

A Note from the Clinic

Structures of organic molecules, whether 2D or 3D, can be intimidating. However, understanding the shape of organic molecules is incredible important. Minor differences among isomers can lead to vastly different properties. Enantiomers, while sharing many physical properties, interact with receptors differently. A classic example is given on page 433 of your text in the health note. Caraway seeds help give the rye bread its unique taste and smell. How different are the smells of rye bread and spearmint? Just think, that difference is due to one chiral carbon. Many pharmaceuticals are chiral compounds with one enantiomer being the biologically active compound. Sometimes the other compound is inactive, but other times, it is biologically dangerous, such as in the case of thalidomide. Being able to visualize structures will help greatly in Modules 11 and 12 as you learn about biochemistry.

Background:

Chemists represent molecules in a variety of ways. For some time now, you have been using **chemical formulas** in order to convey the identity and number of atoms in a given compound. More recently, in the organic chapters, you became acquainted with **structural formulas** where not only are the atoms and number of atoms represented, but their connectivity is given as well. While both of these types of formulas are used widely in chemistry, neither tell the reader how molecules occupy space; that is, neither tell how molecules actually look.

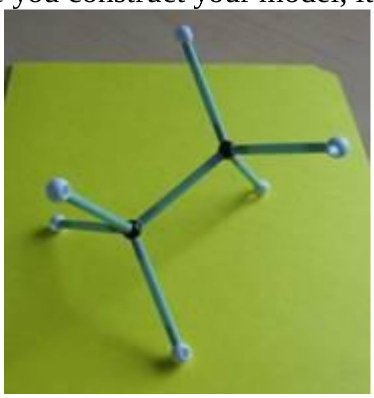
To overcome this shortcoming, chemists have long turned to **molecular models**. You may be familiar with ball-and-stick models where balls of different colors that represent different atoms are connected to one another via sticks that represent bonds. With the advent of personal computers, molecular modeling was taken one step further whereby software programs could be used to show molecules in three dimensions. A relatively simple program called CHIME allows users to not only view molecules in 3-D, but to also spin, zoom, and otherwise manipulate molecules saved in a special format.

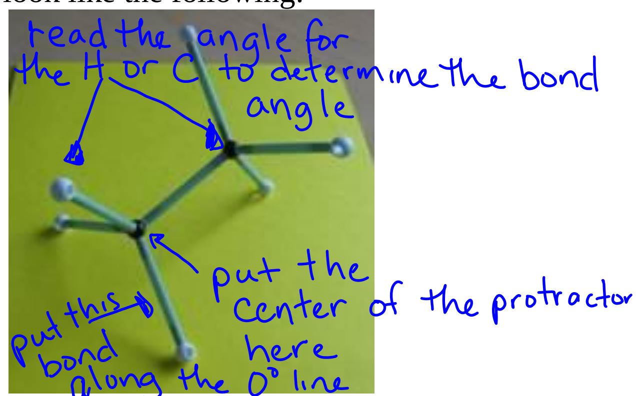
For this lab, you will be exploring molecules with a molecular modeling kit. You will be building (using the model kit included in the Lab Kit) a variety of simple molecules and making observations on their structure. Your task will be to develop a better understanding of molecules and their 3-D properties.

Procedure:

1) Get out the molecular modeling set from your Lab Kit. It should be in a Zip-loc bag.
2) Construct a model of methane, CH_4. Use the black atoms to represent C, the white atoms to represent H, and the green or gray tubes for your bonds. You will need 1 black atom, 4 white atoms, and four green/grey tubes. Once you construct your model, it should look like the following:

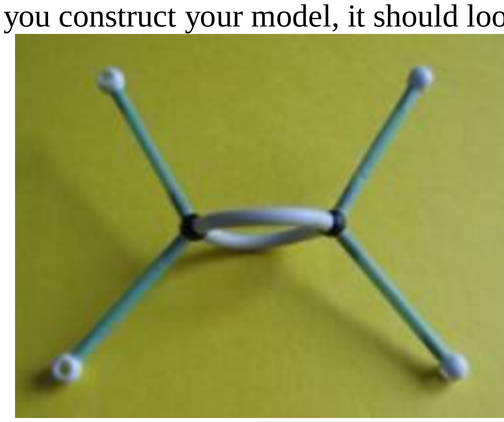
3) To build ethane (CH_3CH_3), replace one of the white atoms with a black (carbon) atom. Use three tubes and three white atoms to add the hydrogens to the new carbon atom. Once you construct your model, it should look like the following:





Using your protractor, measure the H-C-C bond angle, which is the angle made up of one white atom connected to the black atom connected to the second black atom. Also measure the H-C-H bond angle, which is the angle made up of one white atom connected to the black atom connected to a second white atom. Record the values for both these angles.

4) Construct a model of ethene (ethylene), C_2H_4. Start with the ethane model you constructed. Remove one white (hydrogen) atom and tube from each black (carbon) atom. Remove the grey/green tube from between the two black atoms. Now there are two open prongs on the two black atoms. Use two white tubes to make the double bound between the two black atoms. Measure the H-C-C and H-C-H bond angles, as above, and record the values. Once you construct your model, it should look like the following:

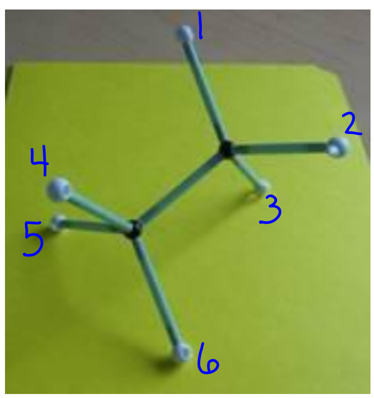


5) Construct a model of ethyne (acetylene), C_2H_2. Start with the ethene model you constructed. Remove one white (hydrogen) atom and tube from each black (carbon) atom. Use one white tube to connect the open prong on the black atoms to complete the triple bond. Measure the H-C-C bond angle, as above, and record the value. Once you construct your model, it should look like the following (note the third white tube is hidden behind the top tube in the photo below):

*Question #1: **(2 points)** Using your protractor measurements, fill in the following chart.*

	Ethane, CH_3CH_3	Ethene, C_2H_4	Ethyne, C_2H_2
H-C-H Bond Angle			N/A
H-C-C Bond Angle			

6) Go back to step 3 and make two models of ethane. Notice how there are six hydrogens (white atoms) in ethane.



Replace the hydrogen (white) atom labeled **1** in one of the ethane models with a bromine (blue) atom to form bromoethane, CH_3CH_2Br. Now, do the same thing with the second model, but replace the hydrogen (white) atom labeled **2** with a blue atom. Are your two models representing the same molecule or are they different molecules? To decide, you need to rotate the molecule and even the single bonds (single bonds are free to spin around) to see if you can make the two molecules look exactly alike. You can do anything to the models but actually break bonds. Rotate, flip, and spin until you either make them look exactly alike or decide there is no way you can make them look exactly alike. If you can make them look exactly alike, then they are the same molecules. If you cannot make them look exactly alike, then they are isomers of each other (see Types of Isomer Powerpoint for more discussion of the different types of isomers). Each isomer is considered a unique molecule. If you made the same molecule when you switched the hydrogens labeled **1** and **2**, then the hydrogen atoms labeled **1** and **2** are considered equivalent. If you made isomers when you switched the hydrogens labeled **1** and **2**, then the hydrogen atoms labeled **1** and **2** are considered non-equivalent.

Take one of the models of bromoethane, convert it back to ethane, then switch the remaining hydrogen (white) atoms (labeled **3-6**) one at a time. Compare the structures again to see if they are the same or different. How many unique structures of bromoethane can you construct? Are all hydrogens (**1-6**) equivalent to one another? If you only can make one unique structure of bromoethane when you compare switching each of the six different hydrogens in ethane, then all six of the hydrogens are considered equivalent, and if you make more than one unique structure of bromoethane, then all six of the hydrogens are not equivalent.

Question #2: ***(3 points)*** *How many unique structures of bromoethane did you find? Draw each of the unique structures. If you have more than one unique structure, you have isomers. Indicate whether the structures are structural, geometric, or stereoisomers. NOTE – if you have 3 unique structures (A, B, and C), then you will have three pairs (A & B, A & C, B & C) to state the relationship between.*

You can make simple structures using the symbol - / | \ and the space bar.

```
   H H
    |  |
H-C-C-H
    |  |
   H H
```

The easiest way to make a structure such as the one of ethane above is to start with the line that contains the carbons. Make this line first, then use the space bar to position the H's and |'s to where you want them for the other bonds. If you have trouble with this, you can always hand-draw your structures and either scan them.

Question #3: ***(1 point)*** *Would you consider all six hydrogen atoms of ethane to be equivalent? Why or why not?*

7) You should repeat the procedure you did to determine how many unique structures of bromoethane to determine how many unique structures of dibromoethane ($C_2H_4Br_2$) exist. Now remember that bromoethane has a molecular formula of C_2H_5Br, so that you will start by labeling the five bromines **1-5**. Then proceed to replace the hydrogen (white) atom labeled **1** by a bromine (blue) atom, to form dibromoethane. Take a second model of bromoethane that is identical to the first bromoethane you started with, and replace the hydrogen (white) atom labeled **2** with a bromine (blue) atom. Compare the two structures. Are they the same or are they different? Continue to do this until you have switched all five of the hydrogens. How many unique structures of dibromoethane can you construct? Are all five hydrogen atoms equivalent?

Question #4: ***(3 points)*** *How many unique structures of dibromoethane did you find? Draw by computer or by hand each of the unique structures like you did for Question 2. If you have more than one unique structure, you have isomers. Indicate whether the structures are structural, geometric, or stereoisomers. NOTE – if you have 3* *unique structures (A, B, and C), then you will have three pairs (A & B, A & C, B & C) to state the relationship between.*

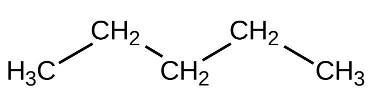
Question #5: ***(1 point)*** *Would you consider all five hydrogen atoms of bromoethane to be equivalent? Why or why not?*

8) Rebuild two ethene molecules as stated in step 4. Note that ethene (C_2H_4) has four hydrogens. Label them 1-4. Now, two hydrogens will be replaced at a time. For the first model, replace the two of the hydrogen (white) atoms labeled **1** and **2** with two bromine (blue) atoms to form dibromoethene. For the second model, replace the two of the hydrogen (white) atoms labeled **1** and **3** with two bromine (blue) atoms to form dibromoethene. Compare the two structures. Are they the same or are they different? Make this comparison for all four hydrogens in ethene by building additional models with the bromines at the positions labeled **1** and **4, 2** and **3, 2** and **4,** and **3** and **4**. How many unique structures of dibromoethene can you construct? Are all of four hydrogen atoms equivalent?

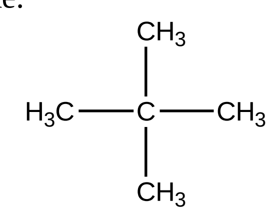
Question #6: ***(3 points)*** *How many isomers of dibromoethene did you find? Draw or type each of the unique structures like you did for Questions 2 & 4. If you have more than one unique structure, you have isomers. Indicate whether the structures are structural, geometric, or stereoisomers. NOTE – if you have 3 unique structures (A, B, and C), then you will have three pairs (A & B, A & C, B & C) to state the relationship between.*

9) Construct a model of normal pentane (C_5H_{12}). You need five black (carbon) atoms, twelve white (hydrogen) atoms, and 16 green/grey tubes. Connect the five black (carbon) atoms with the tubes so that they are in a straight chain. Fill in the open prongs on the black atoms with green/grey tubes and white (hydrogen) atoms. Write the complete and condensed structural formulas of pentane.

10) To examine the differences in boiling points and melting points that can exist between structural isomers, you will look up the boiling points and melting points for two isomers of pentane, normal pentane and neopentane.



normal pentane



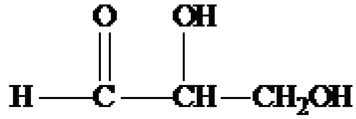
neopentane

This information may be found in a chemical handbook or at ChemFinder.com (URL http://chemfinder.cambridgesoft.com/) or at ChemID Plus Lite (URL http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp). (You may want to make a note of these sites if you ever need to look up information about chemicals.)

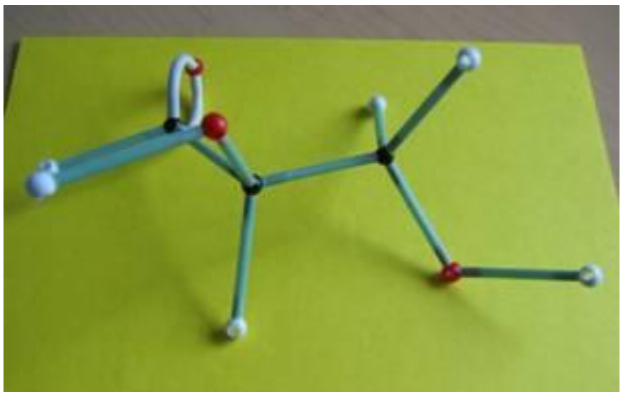
Question #7: ***(2 points)*** *Fill in the following chart for two isomers of C_5H_{12}.*

	Normal Pentane	Neopentane
Melting Point		
Boiling Point		

11) Construct a model of glyceraldehyde, $C_3H_6O_3$:



You will need three black (atoms), three red (oxygen) atoms, six white (hydrogen) atoms, ten green/grey tubes, and two white tubes. Connect the molecule based on the structure above, (one of the isomers is shown in the photo below). Which isomer did you construct, the D or the L (see Timberlake for help)? Construct the other isomer, leaving your original isomer intact. What type of isomers (structural, geometric or stereoisomers) are they?



Question #8: ***(1 point)*** *Which isomer (D or L) of glyceraldehyde did you initially make? Explain how you made your determination.*

Question #9: ***(1 point)*** *What type of isomers were your two glyceraldehydes structures? Explain your reasoning.*

Question #10: ***(1 points)*** *What did you learn about the 3-D shapes of molecules in this lab?*

Question #11 ***(1 point)*** *Give one example of how the 3-D shapes of molecules play a role in their interactions with biological systems.*

Question #12: ***(1 point)*** *Please give constructive feedback regarding this lab. Was it worthwhile? Did it illustrate CHE 106 concepts? What did you gain/learn from doing the lab that you did not learn from the text alone? What would you keep/recommend in future semesters? What would you change? Did you like building models? Why? What other information would you like to convey to your instructor with respect to the use and worth of this lab?*

You should write your answers into a word processing program and save the file either as a Rich Text Format (.rtf) or html file. Then go into the drop box for Lab #7 and cut and paste the answers to each question in the appropriate space. Type your structures as separate .html, .rtf or .pdf files for Questions 2, 4 and 6 and submit to the appropriate drop box OR scan your neatly drawn structures to separate pdf files for Questions 2, 4 and 6 and submit to the appropriate drop box.

Labs not submitted in the appropriate area will *not* be graded.