Laboratory: 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, 8th 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 .docx file.

For questions 2, 3, 4 & 9 neatly hand-draw the structures and then take a picture of *your drawing* and save as a .jpg file. For questions 6 & 7, take a picture of your built molecule and save as a .jpg file.

Go into the Lab – Organic Molecules Report and cut and paste the answers and/or upload images to each question in the appropriate space. (Lab – Organic Molecules Report can be found on the Content page or under Assignments → Quizzes.)

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 (this includes drawings. Everyone is to do their own drawings). At the beginning of each question you should note that you worked with a partner by writing "Lab Partner (fill in name)."

Materials:

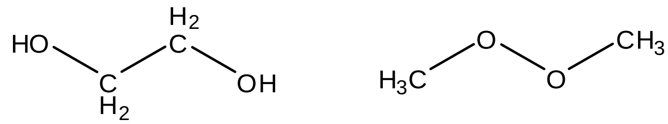
- Model kit (purchase from Parkland Bookstore)
- Protractor (to measure angles): If you do not have a protractor at home, a quick Google image search on "protractor" should yield many pictures of protractors. You can print one off to use, but it is recommended that you make the picture fairly small – no bigger than half a page.

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)

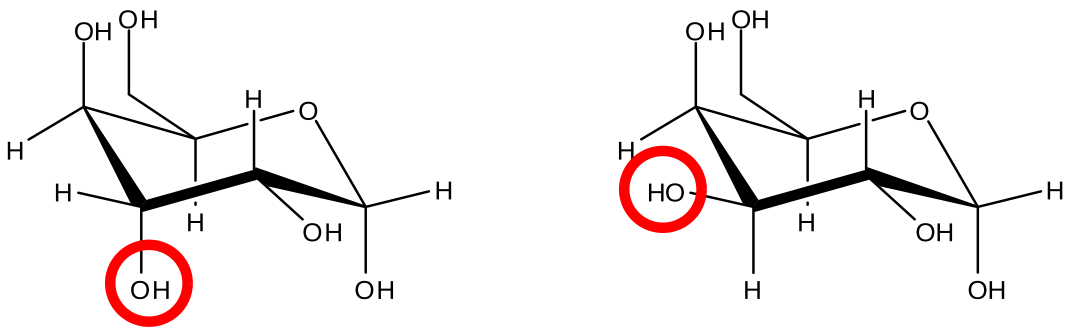
A Note from the Clinic

Structures of organic molecules, whether 2D or 3D, can be intimidating. However, understanding the shape of organic molecules is incredibly important. Minor differences among isomers can lead to vastly different properties. For example, 1,2-ethanediol (ethylene glycol) and one of its structural isomers, dimethyl peroxide. Ethylene glycol is used for antifreeze, has a boiling point of 179 °C, and while it is a poison when ingested, is not explosive. Dimethyl peroxide has a boiling point of -30 °C, and may explode from heat, shock or friction.



1,2-ethanediol **dimethyl peroxide**

Another example would be glucose & galactose. These sugars are geometric isomers, with only a small structural difference in the position of one of their OH groups. See page 445 in Timberlake for more information about these sugars.



glucose **galactose**

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.

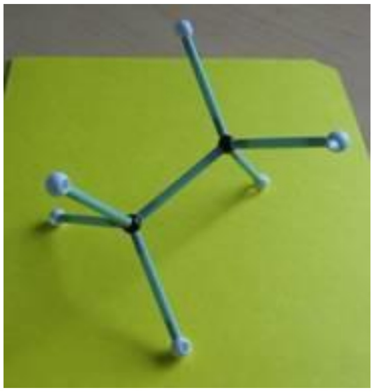
For this lab, you will be exploring molecules with a molecular modeling kit. You will be building (using the model kit purchased from the bookstore) a variety of simple molecules and making observations on their structure. Your task will be to develop a better understanding of molecules and their 3-D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

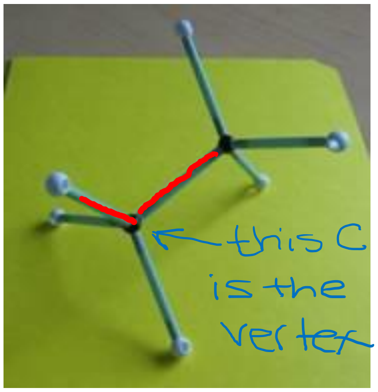
Procedure:

1) Get out the Molecular Modeling kit that you purchased from the bookstore. 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 picture on the right.

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. See the "Lab Equipment Video" (in the Introduction & Getting Started folder) for a demonstration on how to use a protractor. The demo is at about the 9:20 mark of the video. Once you've measured the H-C-C bond angle, 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.

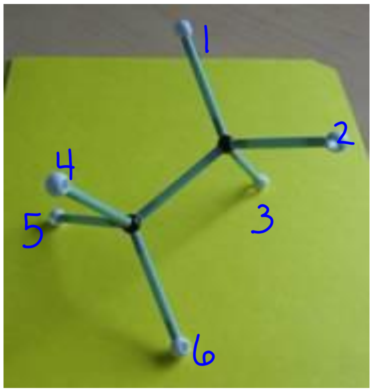
4) Construct a model of ethene (ethylene), C_2H_4. Start with the ethane model you constructed. Remove one white (hydrogen) atom and tube from each black (carbon) atom. Remove the grey/green tube from between the two black atoms. Now there are two open prongs on the two black atoms. Use two white tubes 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 picture on the right.

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 (see picture below). 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 instead, replace the hydrogen (white) atom labeled **2** with a blue atom (instead of the **1** spot) to still make bromoethane, CH_3CH_2Br. 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.

Take one of the models of bromoethane, convert it back to ethane, then switch the remaining hydrogen (white) atoms (labeled **3-6**) to bromine (blue) 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?

See the following videos listed in the Instructions for help:

- Lab 7 help video: https://www.youtube.com/watch?v=VACrh-93HSg.
- Single bond rotation video: https://www.youtube.com/watch?v=ZnSVSQYInAM
- Rotation around single but not double bonds animation: https://www.youtube.com/watch?v=twBagonrMLQ

*Question #2: **(2 points)** How many unique structures of **bromoethane** did you find? **Draw** by hand the expanded structural formula for each of the unique structure(s). If you have more than one unique structure, you have isomers. Indicate whether the structures are structural or geometric isomers. 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.*

Draw the expanded structural formulas by hand and then take a picture of your drawings.

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 hydrogens **1-5** (because the 6th atom is a bromine) 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?

*Question #3: **(3 points)** How many unique structures of **dibromoethane** did you find? **Draw** by hand the expanded structural formula for 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 or geometric isomers. 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.*

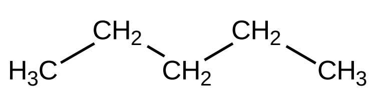
8) Rebuild two ethene molecules as stated in step 4. Note that ethene (C_2H_4) has four hydrogens. Label them 1-4. Now, two hydrogens will be replaced at a time. For the first model, replace two of the hydrogen (white) atoms labeled **1** and **2** with two bromine

(blue) atoms to form dibromoethene. For the second model, replace 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?

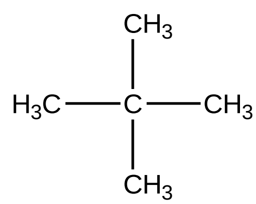
*Question #4: **(3 points)** How many isomers of **dibromoethene** did you find? Draw by hand the expanded structural formula for each of the unique structures like you did for Questions 2 & 3. If you have more than one unique structure, you have isomers. Indicate whether the structures are structural or geometric isomers. 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) Now, convert your structure to neopentane. The structures of pentane & neopentane are given below.



normal pentane



neopentane

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 the two isomers of pentane that you built: normal pentane and neopentane.

This information may be found in a chemical handbook or at ChemSpider.com (URL http://www.chemspider.com/) or PubChem (URL https://pubchem.ncbi.nlm.nih.gov/). (You may want to make a note of these sites if you ever need to look up information about chemicals.)

*Question #5: **(1 point)** Fill in the following chart for two isomers of C_5H_{12}.*

	Normal Pentane	Neopentane
Melting Point		
Boiling Point		

11) So far in this lab, you've explored the alkane, alkene, alkyne & haloalkane functional groups. Use your textbook to identify another functional group (not one of the ones previously explored), and then use your model kit to build an example molecule that contains the functional group you chose. What is the functional group you chose? What is the formula of the molecule? What is the name of the molecule? Would you expect the molecule to be polar or non-polar? Would you expect the compound to have hydrogen bonding?

NOTE: The model kit provides carbon (black), hydrogen (white), oxygen (red) and nitrogen (blue) atoms.

Question #6: ***(2 points)*** *What functional group did you choose? What is the name of the molecule you built? Is the molecule polar or non-polar? Does the compound have hydrogen bonding? Take a picture of the molecule you built.*

12) Choose a second functional group (not one of the ones previously explored), and then use your model kit to build an example molecule that contains the functional group you chose. What is the functional group you chose? What is the formula of the molecule? What is the name of the molecule? Would you expect the c to be polar or non-polar? Would you expect the compound to have hydrogen bonding?

Question #7: ***(2 points)*** *What functional group did you choose? What is the name of the molecule you built? Is the molecule polar or non-polar? Does the compound have hydrogen bonding? Take a picture of the molecule you built.*

13) Predict which of your compounds you expect to have a higher boiling point.

14) Look up the boiling point of each compound.

Question #8: ***(2 points)*** *Which compound do you predict to have the highest boiling point? Explain your prediction based on the structure of each compound. Give the boiling pts for each compound. Do the actual boiling points match your predictions?*

12) Determine how many structural isomers of C_3H_8O exist. Use your model kit to construct one isomer, then try to rearrange the atoms in as many ways as possible. Draw the complete & condensed structural formula for each isomer.

Question #9: ***(2 points)*** *How many structural isomers of C_3H_8O exist? Draw by hand the condensed structural formula of each isomer, like you did in Questions 2, 3 & 4.*

Question #10: ***(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 .docx file.

For questions 2, 3, 4 & 9 neatly hand-draw the structures and then take a picture of *your drawing* and save as a .jpg file. For questions 6 & 7, take a picture of your built molecule and save as a .jpg file.

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