Experiment 3 – Molecular Models and Isomers

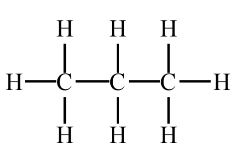
For beginning students in organic chemistry, it usually takes some practice to visualize molecules in three dimensions. It also takes practice to recognize and understand the many possible ways of drawing or representing the same molecule. The purpose of this lab is to construct models of alkanes and haloalkanes and view their three dimensional structures. We will also be constructing models of isomers and observing how they differ in structure and three-dimensional shape. There will also be some naming practice.

Alkanes are <u>saturated</u> hydrocarbons. They are hydrocarbons because they contain only carbon and hydrogen, and they are called saturated because there are no multiple bonds present – the molecule is "saturated" with hydrogen atoms. (It is not possible to add any more hydrogen atoms to the molecule.) Cycloalkanes are alkanes containing a ring of carbon atoms connected together. Haloalkanes are molecules that contain carbon, hydrogen, and one or more halogen atoms (F, Cl, Br, or I) with no multiple bonds in the molecule.

Remember when you are drawing structures that a carbon atom will always form four bonds, a hydrogen atom will form one bond and can never be a "central atom", and a halogen atom will form one bond and have three lone pairs of electrons.

To practice visualizing the three-dimensional structures of organic compounds, it is helpful to build models of the molecules using a molecular model kit. Ball-and-stick model kits contain wooden or plastic balls representing atoms, with a different color for each element, and wooden or plastic sticks that represent bonds. Springs may be used to represent double or triple bonds.

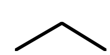
Models are useful because a Lewis structure as it is drawn on paper is not a good three-dimensional representation of a molecule. There are various types of formulas that one can write for a particular molecule. The **complete structural formula** shows all of the atoms and exactly how they are connected. (However, the complete structural formula, as it is drawn on paper, doesn't give you much three-dimensional information.) The **condensed structural formula** is somewhat abbreviated. Atoms are grouped and every bond is not explicitly shown, but the connections between atoms are implied based on how it is written. The **zigzag formula** is even more abbreviated: carbon atoms are assumed to be at the ends and at each bend in the structure, and hydrogen atoms are not even shown, but implied. The assumption is that each carbon makes four bonds, so if one bond is shown for a particular carbon atom, it is implied that three hydrogen atoms are also bonded to that carbon (to make a total of four bonds). The **molecular formula** does not give any structural information. It just specifies the total number of each type of atom present in the compound. Shown below are various formulas for propane.



Complete Structural Formula

$CH_3CH_2CH_3$

Condensed Structural Formula



Zigzag or Line Formula

C_3H_8

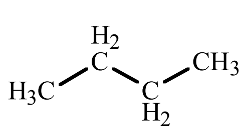
Molecular Formula

The names of alkanes are based on the name of the longest continuous chain of carbon atoms in the molecule. Any substituents present are given a number to indicate their location on the molecule. See your textbook for the IUPAC nomenclature guidelines. The names and formulas of some common alkanes are shown in the table below.

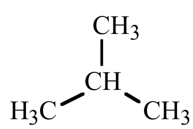
Name	Condensed Structural Formula
Methane	CH_4
Ethane	CH_3CH_3
Propane	$CH_3CH_2CH_3$
Butane	$CH_3CH_2CH_2CH_3$
Pentane	$CH_3CH_2CH_2CH_2CH_3$
Hexane	$CH_3CH_2CH_2CH_2CH_2CH_3$
Heptane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
Octane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
Nonane	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
Decane	$CH_3CH_2CH_2$ $CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

For most organic compounds, if the atoms are arranged differently, a different compound results. Molecules which have the same molecular formula and different structures are called **structural isomers** of each other. Isomers are different molecules with different properties (such as melting point and boiling point) and different names.

For methane (CH_4), ethane (C_2H_6), and propane (C_3H_8), in each case there is only one possible way of arranging the atoms that satisfies the bonding requirements of all of the atoms (each carbon must have four bonds and each hydrogen must have one). However, for butane (C_4H_{10}), there are two possible ways of arranging the atoms. The first is to have all of the four carbon atoms connected in an unbroken line. This is called "n-butane". The second is to have three carbons in a sequence with another carbon attached to the middle carbon. The common name for the second molecule is "isobutane". The structures of n-butane and isobutane are shown below. Note that since the two molecules have the same molecular formula and different structures, they are considered isomers of each other.



n-Butane

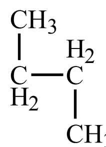
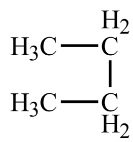
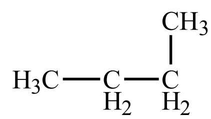


Isobutane

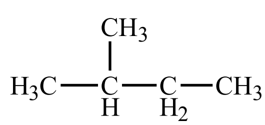
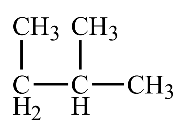
Procedure

1. Using an organic model kit, construct a model of methane. In most model kits, carbon atoms are black, and hydrogen atoms are yellow or white. Turn the structure on its side. Observe that all of the bond angles are equivalent. (This shape is called **tetrahedral**.)
2. Draw a representation of the three-dimensional shape of methane. Draw the complete structural formula and the condensed structural formula.

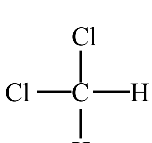
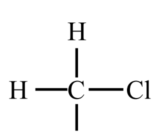
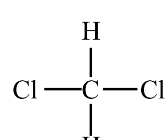
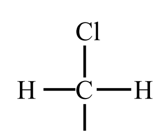
3. Make a model of ethane and of propane. Notice that all of the bond angles are equivalent for each molecule. Draw the complete structural formula and the condensed structural formula for each molecule.
4. Make a model of n-butane. Notice that in the three-dimensional structure, the carbons are not actually in a straight line. Draw the complete structural formula and the condensed structural formula for butane.
5. Using your model of butane, rotate the bonds and twist the molecule. There is free rotation around single bonds, so molecules are constantly twisting, rotating, and changing their **conformation**. It is important to understand that this type of motion is happening constantly in any given sample. Thus, the following structures represent the <u>same</u> molecule in different conformations. You should be able to recognize that these structures are equivalent and represent the same molecule. They are NOT isomers of each other!
6. Make a model of isobutane (the IUPAC name for isobutane is 2-methylpropane). Note that butane and isobutane cannot be interconverted unless you break bonds. They thus represent distinct molecules with different properties. Draw the

complete structural formula and the condensed structural formula for isobutane.
7. Find a chemistry handbook or catalog in the lab (you may need to ask for one at the stockroom). Look up the molar mass, melting point, boiling point, and density for butane and for isobutane (which might be listed as 2-methylpropane).
8. There are three isomers for C_5H_{12}. Make a model of each isomer. For each isomer, write the condensed structural formula and name it. Look up the molar mass, melting point, boiling point, and density for each isomer.
9. Construct models of cyclopropane, cyclobutane, and cyclopentane. You will need to use springs instead of sticks for the carbon-carbon bonds in the first two molecules, because their bond angles are significantly different from the normal 109.5°. Cyclopropane and cyclobutane have a significant amount of "ring strain." Draw the full structural formula, the condensed structural formula, and the geometric formula for each.
10. Make models of the following molecules and convince yourself that they are equivalent.

11. Starting with a model of methane (CH_4), remove one hydrogen atom and replace it with a chlorine (green) atom. You have made a model of CH_3Cl (chloromethane). Does it matter which hydrogen is replaced?
All hydrogen atoms in CH_4 are considered <u>equivalent</u>. Each one has the same angle and position relative to the other hydrogen atoms in the molecule. Each one is equidistant from all of the others. Look carefully at your model to convince yourself of this.
12. Again starting with a model of CH_4, make a model of CH_2Cl_2 (dichloromethane). To do this, remove two hydrogen atoms and replace them with chlorine atoms. Are there different isomers possible for this formula?
Given the structures below: are these molecules <u>isomers</u> or <u>equivalent</u>? Explain.

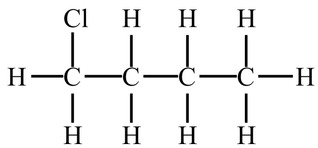
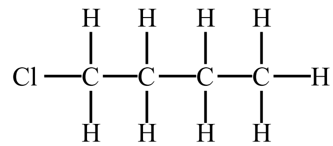
13. Go back to your model of ethane, CH_3CH_3. Are all of the hydrogen atoms equivalent? Explain. Draw the three-dimensional structure of this molecule.
14. Starting with your model of ethane, make a model of chloroethane, CH_3CH_2Cl. Again, do this by removing one of the hydrogen atoms and replacing it with a chlorine atom. Are there different isomers possible for this molecule? Explain. Draw the three-dimensional structure of this molecule.
15. Look at your model of chloroethane. In this molecule, the hydrogen atoms are <u>not</u> equivalent. Two of the hydrogen atoms are closer to the chlorine atom, and the other three hydrogen atoms are further away from the chlorine atom. You will now make a model of dichloroethane by removing another hydrogen atom from the molecule and replacing it with a chlorine atom. However, there are two possible locations for the second chlorine atom. It could be placed on the same carbon as the first chlorine atom, or it could be placed on the other carbon atom. Thus, there are two isomers possible for the molecular formula $C_2H_4Cl_2$. Make models of both isomers and compare them.

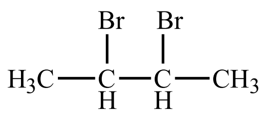
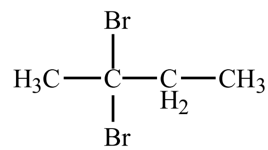
    It is important to notice that there are <u>only</u> two isomers possible for this molecule. There are five possible locations for the second chlorine atom, but since two of the positions are equivalent to each other, placing the chlorine at either of these two positions results in the same molecule, because there is free rotation around the bonds in this molecule. Similarly, the other three positions are equivalent to each other, so placing the chlorine at any of these positions will give you the same molecule. <u>Convince yourself of this by making various models of the different possibilities and noticing which ones are the same.</u> Therefore, even though there are five possible locations for the chlorine, there are only two **types** of positions, so only two isomers are possible.

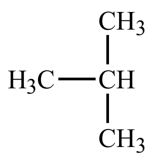
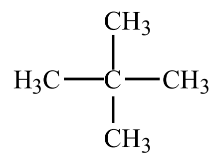
    Draw the two isomers. One of them is named 1,1-dichloroethane and the other one is named 1,2-dichloroethane. Write the appropriate name near each structure.
16. How many isomers are possible for the molecular formula $C_3H_6Cl_2$? Draw and name each isomer. Make models of the molecules. Make sure that all of the isomers you list are actually <u>different</u> molecules.

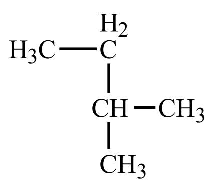
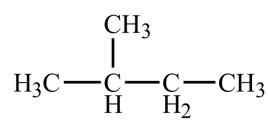
<u>Questions</u>

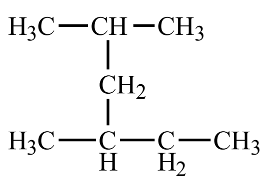
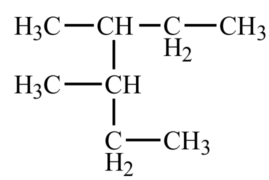
1. For each of the following pairs of molecules, state whether they are isomers, identical, or neither. Briefly explain your reasoning in each case.

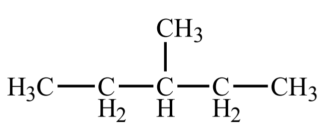
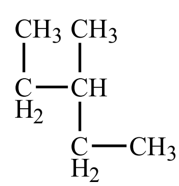
a.  and 

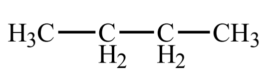
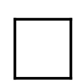
b.  and 

c.  and 

d.  and 

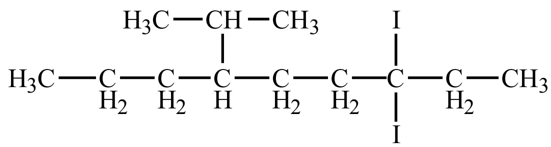
e.  and 

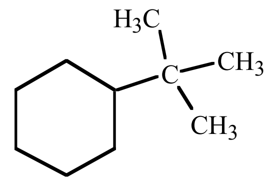
f.  and 

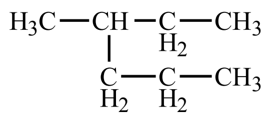
g.  and 

2. Name each of the molecules in question #1 above.

3. Name each of the following molecules.







4. Draw condensed structural formulas for:

   3-ethylpentane

   1-bromo-3-chlorocyclopentane

   1,2-dibromobutane

   methylcyclohexane

5. Write the condensed structural formulas for all isomers of C_4H_9Br. Name each isomer.

6. Write the condensed structural formulas for all isomers of C_6H_{14}. Name each isomer.