EXPERIMENT

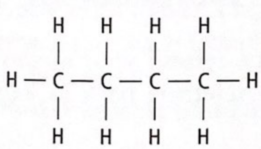
# 15A

# Making Models of Some Carbon Compounds

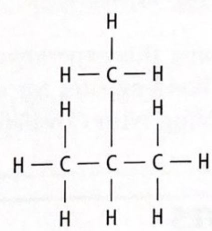
The term structure in chemistry refers to the way in which the atoms of a molecule are joined together. Chemists can often predict the physical and chemical properties of a substance if its structure is known; hence, it is important to find a way of representing that structure. In two dimensions, the most common representations are the electron-dot (Lewis) formula, in which all the valence electrons of the atoms are shown, and the structural formula, in which bonding pairs of electrons are shown by a single line and non-bonding electrons are usually left out. These are useful up to a point, but as the molecules get more complex it is important to show the three-dimensional nature of the molecule. This is where ball-and-stick, ball-and-spring, or space-filling models help in the visualization.

Substances having the same molecular formula but a different structural formula are said to be *isomers* of one another; they are exhibiting *isomerism*. Two categories will be considered here, *structural isomers* and *geometric isomers*.

Carbon compounds often give rise to a number of different structural isomers because the carbon atoms can combine with each other in a variety of ways, including chains and ring structures (cyclic compounds). For example, the hydrocarbon butane, $C_4H_{10}$, may exist with its four carbon atoms linked in a straight chain of four or in a branched chain consisting of three carbons in a row, with the fourth attached to the central carbon.

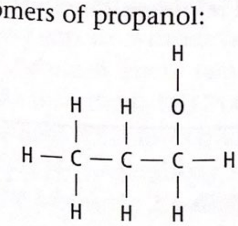


n-butane

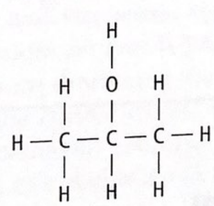


2-methylpropane (isobutane)

Other types of structural isomers occur when the carbon skeleton is identical, but the position of a functional group attaches to the carbon skeleton at different positions. Note the placement of the OH group in each of the following isomers of propanol:

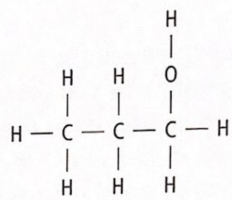


1-propanol

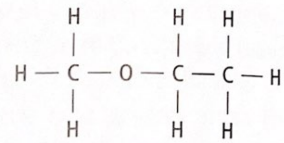


2-propanol

Sometimes, the two structural isomers may belong to two totally different classes of compounds, even though they have the same molecular formula. As a result they may have very different physical and chemical properties. For example, the following two isomers with molecular formula $C_3H_8O$ belong to two different classes of compound, one in which the oxygen atom is attached to a hydrogen atom (an alcohol) and one in which the oxygen is attached between two carbon atoms (an ether):

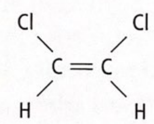


1-propanol

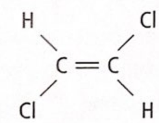


methoxyethane (methyl ethyl ether)

Geometric isomerism occurs in some molecules having at least one double bond. The sequence for the atoms and bonds in the molecule is the same for each isomer, but there is a different orientation of the atoms or groups attached to the carbon atoms in the double bonds. Since rotation about a double bond is restricted, the parts of the molecule on either side of the double bond remain in fixed positions. In order to have this type of isomerism, each carbon atom in the double bond must have two different groups attached to it. The compound 1,2-dichloroethene exhibits this kind of isomerism:



cis-1,2-dichloroethene
(both chlorines are on the same side of the double bond)



trans-1,2-dichloroethene
(the two chlorines are on opposite sides of the double bond)

Before doing this experiment, if necessary, refresh your memory as to the number of bonding sites for each atom by referring back to Experiment 9B (Model Building With Covalent Molecules).

## OBJECTIVES

1. to construct molecular models of some simple organic substances and to represent these structures with electron-dot and structural formulas
2. to construct molecular models of more complicated organic substances illustrating different types of isomers and represent them with structural formulas

## SUPPLIES

**Equipment**
molecular model kit

## PROCEDURE

1. Using the type of molecular model kit your instructor has made available to you, construct models for each of the following alkanes. Then, in your notebook, draw the structural formula and electron-dot formula for each molecule.
   a. methane $CH_4$
   b. ethane $C_2H_6$
   c. propane $C_3H_8$
2. Construct models for all structural isomers you find for each of the following compounds. Draw the structural formulas for all isomers and name them.
   a. butane $C_4H_{10}$
   b. pentane $C_5H_{12}$
   c. hexane $C_6H_{14}$
   d. cyclohexane $C_6H_{12}$
3. Construct models for all structural isomers of butene, $C_4H_8$. Draw the structural formulas for all isomers and then name them. Remember to consider the possibility of geometric isomerism.
4. Construct models for all structural isomers of propyne, $C_3H_4$, and butyne, $C_4H_6$. Draw the structural formulas for all isomers and then name them.
5. Construct models for all structural isomers of hexanol, $C_6H_{13}OH$, which have a straight chain of six carbon atoms. Identify the position of the OH group, draw the structural formulas for all isomers, and name them.
6. Construct models for the following structural isomers which have the same molecular formula, $C_2H_6O$. Observe how the different placement of the oxygen atom makes a big difference to the structure. Draw the structural formula for each isomer.
   a. ethanol $C_2H_5OH$
   b. methoxymethane (dimethyl ether) $CH_3OCH_3$

## POST LAB CONSIDERATIONS

It can be seen that even with relatively simple molecules, there are often many structures possible. The IUPAC system for naming organic compounds was introduced so that there would be no confusion as to the name of a compound of a particular structure. Your instructor will give you the rules you will need for the classes of compounds you study. Once you know the rules, the structural formula can be written from the name and vice versa. Many common names for chemicals are in fact shortened versions of their IUPAC names. For instance, the insecticide DDT takes its name from shortening the longer name **d**ichloro**d**iphenyl**t**richloroethane. (Actually the correct IUPAC name is even longer: 1,1-bis(4-chlorophenyl)-2,2,2-trichloroethane!) Likewise the common name for the herbicide 2,4-**d**ichlorophenoxyacetic acid is 2,4-D.

## EXPERIMENTAL RESULTS

Your observations in this experiment may be recorded in table form. However, it will be difficult to prepare the table for Steps 2, 3, 4, and 5 in advance as you do not know how many structures there are for each substance. Just list the compound and then draw all of the structures you find for that compound.

## ANALYSIS OF RESULTS

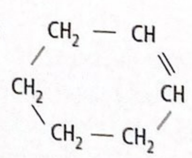
1. How many isomers did you find for each of the following alkanes?
   - **a.** methane
   - **b.** ethane
   - **c.** propane
   - **d.** butane
   - **e.** pentane
   - **f.** hexane
2. Can cyclopentane ($C_5H_{10}$) be considered an isomer of pentane? Explain.
3. Look at your structures for pentane. How many different molecules can be made of pentene, $C_5H_{10}$, by replacing a C–C single bond with a C=C double bond? (Consider the possibility of geometric isomerism.)

## FOLLOW-UP QUESTIONS

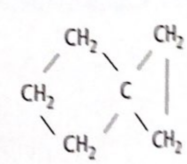
1. Look at the following four molecules, write the molecular formula for each one, and compare the formula. Assume a general hydrocarbon with no double or triple bonds or ring structures has the formula $C_nH_{2n+2}$. Based on what you observed about the formulas of the four molecules, give a set of rules that allow you to predict the number of hydrogen atoms involved in a general hydrocarbon when (a) one or more double bonds is present, (b) one or more triple bonds is present, and (c) one or more ring structures is present.

**A** $H-C\equiv C-CH_2-CH_2-CH_2-CH_3$ **B** $CH_2=CH-CH=CH-CH_2-CH_3$

**C**



**D**



2. Use a reference source to research what trans fatty acids are, how they arise, and what possible health risks may result from ingesting them. Cite the reference source you use.

## CONCLUSION

Explain why there is such a huge number of organic compounds.