Activity 2

Modeling Molecules

**GOALS**
In this activity you will:

- Connect the two-dimensional drawing of a simple organic molecule to the three-dimensional structure it assumes.
- Examine the differences in molecular shape that result from small differences in molecular structure and the differences in properties of substances that can result from these differences in shape.
- Model the chemical reaction that takes place during the soap-making process.
- Predict the structures formed by atoms by examining their bonding (valence) electrons.

**What Do You Think?**
Here are the structures of two different four-carbon molecules that have the same numbers of carbons and hydrogens.

- **Describe the differences in these two molecules’ shapes.**

Record your ideas about this question in your Active Chemistry log. Be prepared to discuss your responses with your small group and the class.

**Investigate**
In this activity, you will use molecular model sets to build some hydrocarbons and other molecules so that you can see what shapes soap molecules take. Understanding the shapes of molecules is crucial to understanding how the molecules interact with each other.
It is these interactions that determine the behaviors of substances. To design a soap that has certain properties, you have to decide what kinds of molecules should be included in the ingredients used to make the soap. Therefore, you have to be able to predict the shapes of molecules.

1. Work individually or in pairs. Open a molecular-model set and organize the balls and sticks in it. What categories of balls and sticks are there?

   a) Write down what information describes each color of a ball. For example, a black ball has four holes that appear to be equally spaced apart. (It can make four bonds.)

2. A hydrogen atom will make 1 bond, an oxygen atom will make 2 bonds, a nitrogen atom will make 3 bonds and a carbon atom will make 4 bonds. (This can be remembered as HONC – 1, 2, 3, 4.)

   a) Which colors in your set could represent each of these elements? Of course, the actual atoms aren’t red or blue or any color at all. The different colors make it easier to keep track of which atoms are where.

3. Use sticks and balls to make a structure consisting of no more than six different balls. Also, make sure that all the holes in the balls have sticks in them that are connected to other balls. If you are able to make a structure, then you have constructed a model of a molecule that could exist.

   a) Sketch a copy of your model in your Active Chemistry log.

4. The covalent bonds formed by these atoms are each composed of an electron pair. Because all electron pairs have a negative electrical charge, they repel other electron parts. You will use strings to model the positions in space of these bonds or electron pairs. Working in a group of four, have one person hold one end of four 20-cm strings in one hand. Each person (including the one already holding all four strings) should take the other end of one string and hold it out away from the center. Try to make each string (or at least its far end) as far away from all the other strings as possible.
5. Now, use the molecular-model set to build a molecule of methane (CH₄) or natural gas, using one carbon atom and four hydrogen atoms from the molecular-model kit. The name of this molecular shape is a tetrahedron. In geometry, a tetrahedron is a four-sided figure in which each side is a triangle.

6. Next, make a two-carbon molecule by joining two carbon atoms together and filling the rest of the holes in the carbon atoms with hydrogen atoms.

   a) Write down the formula of the molecule you have made.

   Now replace one of the hydrogen atoms with another carbon atom, and surround the new carbon atom with hydrogen atoms.

   b) Write down the formula of the molecule you have made. This molecule is propane, the gas used in gas grills.

   Replace a hydrogen atom with another carbon so that you have four carbon atoms in the chain. Add hydrogen atoms as needed.
c) What does the molecule look like? Draw it in your Active Chemistry log. Write down its formula. This compound is called butane, the liquid fuel in most lighters.

7. Make the four-carbon molecule have different shapes by twisting around the center C—C bond.
   a) Draw the two shapes that are the most different in your Active Chemistry log.

8. Now, remove the bond that you twisted around (in the center), and also remove one hydrogen from each of the two middle carbons. Most kits have flexible bonds that can bend for making double bonds. Create a double bond between the two middle carbons with two of those flexible bonds.
   a) Is it possible any more to twist around the center bond?
   b) Draw the shape of the molecule you just made.
   c) Which of the two molecules in What Do You Think? is it like? Which one must be bent and which one can be more like a straight line?
   d) How can you make the other molecule in the What Do You Think? section? Answer this question in your Active Chemistry log.

In the first molecule shown in What Do You Think?, the arrangement of carbons around the double bond is called a cis arrangement. In the second molecule, the arrangement of carbons is called a trans arrangement.

9. Take apart your molecules and begin anew. Build one methane (CH₄) molecule. Start another molecule by beginning a carboxyl group (—COOH), as shown in the diagram. Start by making two bonds (a double bond) between a carbon atom and an oxygen atom. Finish the carboxyl group by attaching another oxygen atom to the carbon, and then a hydrogen atom to that oxygen.

Such a cluster of atoms (—COOH) is called a functional group. The name of this functional group is carboxyl. Molecules that have this functional group attached are called carboxylic acids.

The carbon atom has room for one more bond. Remove a hydrogen atom from the methane molecule you made earlier and attach the carboxyl group at that point. This molecule is acetic acid (the acid in vinegar), CH₃COOH. The carboxyl group makes it an acid.
10. Make a glycerol molecule (used in cosmetics) by connecting three carbon atoms together with single bonds, and then connecting an —OH group to each carbon. Fill in the other empty holes on the carbon atoms with hydrogen atoms.

a) Write the formula for this molecule. Do not take apart this glycerol molecule because you will need it again later.

11. Next, construct a fatty acid by replacing one of the hydrogen atoms in the CH₃ part of your acetic acid (CH₃COOH) model with a carbon atom, then adding another one to that one, and so on, to create a long chain of carbon atoms.

When your molecule contains 18 carbon atoms, you have the backbone for a molecule of stearic acid. You will probably need to combine with another group in order to have enough atoms to use or you may have to stop at a smaller molecule with fewer carbon atoms.

A complete stearic acid molecule is shown in the two diagrams below. (Make sure your larger group keeps one glycerol molecule to use later.) Finally, fill in all the empty holes in the carbon atoms with bonds to hydrogen atoms.

You can see that the molecule you have made can be stretched out in more or less a straight line.

The carbon backbone zigzags back and forth, but the overall shape of the molecule can be more or less linear, as in the drawing below. In this kind of notation, the chain of carbons forms the skeleton or “backbone” of the molecule and the hydrogen atoms form the other bonds on each carbon atom.

Take your molecule and put it on a table next to other stearic acid molecules. Gently push them together. You can see that they can be packed together quite tightly.

12. Take one of the stearic acid molecules and change its structure. Create a cis-double bond between the ninth and tenth carbons in the carbon chain (begin counting at the carboxyl group) by removing a hydrogen atom from each one and connecting them with a second bond. This is cis-oleic acid, a monounsaturated fatty acid. Have your teacher put the oleic acid molecule back in the middle of the pile of stearic acid molecules.

a) How does this affect the way the pile can be packed together?
13. You can model what happens in the saponification (soap-making) reaction.
   a) Describe how three stearic acid molecules can be attached to a single glycerol molecule to create a fat (as shown in the diagram).
   b) In your log, draw this diagram and identify the parts from the original three stearic acid molecules and the single glycerol molecule.

14. When this fat molecule reacts with three NaOH units, three units of soap (shown in the diagram) and one glycerol molecule are created.

15. Describe a skit for the class that could illustrate the saponification reaction. Have different people represent different parts of the soap molecule. (Actually, soap isn’t a molecule. Each unit of soap is two charged ions: a positively charged sodium ion and a long hydrocarbon chain whose oxygen atom at the end carries a negative charge.)
Chemical Structures and Isomers

One of the things chemists want to know about a compound is its chemical structure. The beauty of organic chemistry is the ability of the carbon atom to bond with itself to form very large and very complex structures. A simple hydrocarbon formula such as butane, C₄H₁₀, can represent two different compounds. Such compounds are called **isomers**. You saw this with the models you built in the Investigate section. Each isomer of butane has the four carbons attached in a different arrangement and each will have its own characteristic physical and chemical properties.

Another way to draw isomers is to use “line-bond” drawings. These show only how the carbons are connected to one another. The line-bond drawings do not show the hydrogen atoms and their bonds. Instead, they only show the bonding of the carbon atoms. It is an easy way to quickly draw structures for comparison purposes. (Note: this is only done with carbon atoms.)

A hydrocarbon where all carbons have single bonds is called a **saturated hydrocarbon**. An **unsaturated hydrocarbon** contains one or more carbon-carbon double or triple bonds. (Remember, all carbons must have four bonds!) To convert butane into a simple unsaturated hydrocarbon, C₄H₈, two hydrogen atoms must be replaced with one double bond. The formula C₄H₈ represents four different...
compounds, again each with its own physical and chemical properties. You can see how quickly the number of organic molecules increases when you add more carbon atoms, double bonds, and atoms such as oxygen and nitrogen.

\[
\begin{align*}
\text{cis-2-butene} & : \text{H} \quad \text{trans-2-butene} & : \text{H} \\
\text{1-butene} & : \text{H} \quad \text{2-methylpropene} & : \text{H}
\end{align*}
\]

**Chem Words**

**Lewis structure**: a system of showing chemical structure in which the valence electrons of an atom are placed around the atom. Bonds are shown as a pair of dots or as a line. Non-bonding valence electrons are shown as dots that are not placed between the symbols or elements in the compound.

**Lewis Structures of Atoms and Molecules**

Recalling the octet rule and the special stability attained in filling an electron shell, you can see that a carbon atom (in Group IVA) needs four more electrons. However, carbon almost never gives up electrons or takes on electrons. Because of this, nearly all carbon compounds are covalent and contain four bonds to other atoms. **Lewis structures** are diagrams that show only the outer-shell valence electrons. These are the electrons used in bonding. A look at the Lewis structures in the diagram of some common atoms (H, C, N, O, F) allows you to figure out how many electrons each needs to fully bond and how many bonds it will usually form. Hydrogen requires only two electrons to fill its shell for stability.

\[
\begin{align*}
\text{H} & \quad \text{C} & \quad \text{N} & \quad \text{O} & \quad \text{F}
\end{align*}
\]

Look at a few simple molecules with full electron shells after bonding. The Lewis structures of water and methane would look as shown in the diagram. The hydrogen always has two electrons and the oxygen or carbon has eight electrons.
Active Chemistry

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Shared pairs of electrons between two atoms represent covalent bonds, while unshared pairs of electrons on one atom belong only to that atom. These are called “lone pairs” or “non-bonding pairs.”

One shorthand method for drawing structures uses a single line to represent a single bond. In this fashion, the two molecules can be drawn as shown.

You can draw very complicated structures such as the structure of a fat molecule, in this way. As suggested previously, each atom will form a standard number of bonds, depending on how many valence electrons it has. Carbon always forms four bonds, while nitrogen forms three, oxygen forms two, and the halogens (F, Cl, Br, I), like hydrogen, form one bond. A structural formula of this type tells you the number of each kind of atom and how they are connected to one another. In molecules having polar covalent bonds, you can also deduce the polarity of the molecule by considering its geometry.

**Double and Triple Bonds**

Sometimes two or three bonds can form between two atoms. When double or triple bonds are formed, atoms share more than one pair of electrons. These fall into the unsaturated class of compounds and have their own unique physical and chemical properties. The two simplest of these organic compounds are ethene and ethyne, as shown in the diagram.

Note that the “-ane” ending as in methane (ethane, propane, butane) indicates a saturated hydrocarbon. The “-ene” ending indicates an unsaturated molecule with at least one double bond. The “yne” ending indicates an unsaturated molecule with at least one triple bond. The terms “saturated” and “unsaturated” are in reference to the total number of hydrogen atoms. An unsaturated hydrocarbon has fewer hydrogen atoms than it could have and can react to take on more hydrogens.

You observed during the activity that single bonds allow free 360° rotation about the bond. The result of this is that the molecule can adopt many different shapes. When you made a C=C double bond, you found that it was rigid and could not be rotated without breaking the bond. In the same way, the two carbons of a triple bond cannot be rotated without breaking the bond between them. Compounds with

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**Chem Words**
- **structural formula:** a formula of a molecule that shows not only all of the atoms but also how they are connected to each other.
- **polar covalent bond:** a bond between two atoms of different electronegativity. The center of electron density is found nearer to the more electronegative atom.
double and triple bonds in their structure have more rigid structures than saturated compounds. This generally results in higher melting and boiling points.

One of the most interesting natural unsaturated cyclical compounds to be discovered early on was benzene, C₆H₆. Benzene can be isolated from coal tar and is a known carcinogen. Although the formula was known by 1825, its structure puzzled chemists for decades and many odd structural formulas were proposed. Credit was given to the chemist Friedrich August Kekulé von Stradonitz for being the first to deduce a reasonable structure for this unusually stable unsaturated compound. Although later found to be incorrect, the alternating single and double bonds found in benzene became known as “Kekulé” structures in his honor.

**cis and trans Structures**

In the What Do You Think? section at the beginning of this activity, you were shown two molecules. They had the same formula and name (C₄H₈ and 2-butene), and yet, they were clearly different molecules. The compound on the left is a cis isomer and the other isomer is called trans. Typically, a trans compound will be more stable than the cis isomer. It will pack into a crystalline structure better and have a higher melting point. The trans isomer is more stable than the cis isomer. Therefore, it is less reactive than the cis isomer.

You often hear on television that trans-fatty acids are bad for you and that cis-fatty acids are healthier in your diet. The cis compounds are the natural form of most fats. Enzymes can more easily digest them by breaking them into smaller molecules that your body can use.
The Tetrahedral Carbon

Each carbon bond is made of two shared electrons. As your group discovered by using the four strings representing the four bonds, the molecule takes on the shape of a tetrahedron when the four bonds are positioned to minimize the electrical forces of repulsion of the hydrogen atoms. It is this tetrahedral shape that gives two-dimensional drawings of carbon chains their “zig-zag” appearance. More importantly, the tetrahedral carbon atom provides a multitude of interesting, complex, and useful structures. The specificity of many bio-molecules, such as enzymes, are dependent upon this unique feature of carbon bonding.

What is Soap?

The soaps you made before you began this chapter were produced by a chemical reaction between two ingredients: a naturally occurring animal or vegetable fat, and NaOH, a strong base. The name for this type of reaction is saponification and it occurs between any fat and a strong base. Fats, also called triglycerides, are organic (carbon-containing) molecules produced by living organisms. They are composed of three long hydrocarbon chains, each one attached to one of the three —OH groups on a glycerin molecule by a carboxyl group.

Two ways of drawing the chemical structure of stearic acid

Chem Words

tetrahedron: in geometry, a pyramid with four sides that are equilateral triangles. In chemistry, the term used for molecular structures in which there are four bonds at equal angles (109.5°) around an atom.
saponification: the hydrolysis of triglyceride in the presence of a base.
In the soap-making process, when you mix the fat and the base together, the molecule comes apart, creating glycerin and three unattached fatty acids as products. The fatty acid molecules have a long non-polar hydrocarbon chain and a **carboxylic functional group** on one end. A **functional group** is the characteristic group of an organic molecule.

Under basic conditions, the carboxyl group loses an $\text{H}^+$ ion. The negative ion formed is attracted to the positive sodium ions ($\text{Na}^+$) in the solution. This new ionic compound formed is the soap. One example of a soap compound is shown using the “zig-zag” convention.

Soap has been made this way for thousands of years. Traditionally, the fats used in making soap have been some kind of animal fat like tallow (from beef) or lard (from pork), although vegetable oils like olive or coconut have also been used. You used sodium hydroxide as the base. In the past, wood ashes have been used as the base (also called lye). Other ingredients can be added to change the properties of the soap somewhat, but the basic recipe has not changed much over time.

**What Do You Think Now?**

At the beginning of the activity you were asked to describe the differences between two molecules that have the same numbers of carbons and hydrogens.

You now have made models of the two molecules. Building a model and holding it in your hand is the best way to become familiar with the shape of a molecule. The two molecules are not identical. What is it about the $\text{C}≡\text{C}$ double bond that makes it different from a $\text{C}–\text{C}$ single bond?
Chem Essential Questions

What does it mean?
Chemistry explains a macroscopic phenomenon (what you observe) with a description of what happens at the nanoscopic level (atoms and molecules) using symbolic structures as a way to communicate. Complete the chart below in your Active Chemistry log.

<table>
<thead>
<tr>
<th>MACRO</th>
<th>NANO</th>
<th>SYMBOLIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Describe at least two properties of animal fat that you have observed when cooking or eating beef or chicken.</td>
<td>Describe a fat molecule in terms of its molecular structure.</td>
<td>Draw a structural model for a fat molecule.</td>
</tr>
</tbody>
</table>

How do you know?
What are the types of models explored in this activity? Which model would be the best for predicting the number of bonds an atom will form?

Why do you believe?
Diamond is one of the hardest substances known, so it is very difficult to break. Graphite is so soft and slippery that it is often used as a lubricant. (This property makes it a good writing material, because it helps the point of your pencil slide easily across the paper, leaving a trail of graphite bits behind.) Yet both of these materials are made of only one kind of atom, carbon. What do you think accounts for their differences?

Why should you care?
For the design and presentation of your soap, it will be helpful to have a solid understanding of the process of saponification. Explaining to your company how the soap is formed will assure your boss that you are competent and knowledgeable. Using models in your presentation will help others to understand your vision for the world’s best soap. How will you do this in your presentation?

Reflecting on the Activity and the Challenge
The world is filled with many different compounds. In order to fully understand their differences and produce materials with the properties you want, you have to look at both the macroscopic properties of those compounds and the properties that arise at the atomic level. The ways the atoms are connected and the three-dimensional shape of the molecules contribute to the properties of the material. You can draw diagrams and build models of those atomic structures to better visualize and understand the structures of substances, and in turn, their properties. Understanding the structure of a soap molecule can help you predict how the properties of soaps change as you change the ingredients used to make the soap.
1. Are the shapes of these two molecules different? If so, why?

2. Which of the two molecules in Question 1 has a *cis* arrangement about the double bond, and which has a *trans* arrangement? Explain.

3. Are these two molecules different or the same? Explain.

4. Draw the Lewis structure of each of the following atoms. Use the Roman numeral group number in the periodic table for the number of valence electrons.
   a) N   b) S   c) F   d) Ar

5. Which of the atoms you drew in Question 4 can make bonds and which ones cannot? How many bonds can each one make?

6. a) Draw the Lewis structure of ammonia, NH₃.
   b) Draw the chemical structure of ammonia, showing the bonds as lines.
   c) Would you expect ammonia to be a polar molecule? Explain.

7. The following problems are about ethanol (grain alcohol), CH₃CH₂OH.
   a) Using a line to represent each bond, draw the chemical structure for ethanol.
   b) How many bonds does each carbon atom make? Does carbon always make the same number of bonds? Why?
8. The structure below represents a fat that could be used to make a soap. Draw the chemical structure of one unit of soap in the cis form that would be created by reacting this fat with three units of NaOH.

9. Preparing for the Chapter Challenge

In the Chapter Challenge, you will need to explain the chemical reaction in which soap is made from the ingredients you choose to use. You will need to represent the molecules involved in this chemical reaction. There are different ways to represent a molecule: Lewis diagrams and two kinds of structural diagrams (one with all the C-H bonds shown, and the other without). In your Active Chemistry log, use the glycerol molecule as an example, and represent it in all three ways. It may help to build glycerol first using the molecular-model sets.