Introduction

A group of atoms held together by covalent bonds is called a *molecule*. Although we represent molecules on paper as being two-dimensional for convenience, they are actually three-dimensional. By building molecular models, chemists come to understand the bonding, shapes, and polarity of even the most complex molecules. A molecule can be represented on paper by either a molecular or a structural formula. A molecular formula indicates the number and kind of each atom present in a molecule. Some familiar molecular formulas are shown below.

\[
\begin{align*}
\text{NH}_3 & \quad \text{CH}_4 \\
\end{align*}
\]

The molecular formulas do not provide any information concerning the actual arrangement of atoms in a molecule. Such information is given by structural formulas such as the following.

\[
\begin{align*}
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{H} \\
\end{align*}
\]

These structural formulas are two dimensional. The angles shown are not true to the shape of the molecule. Structural formulas can be made to convey more information by using the following symbolism.

- for a bond in the plane of the paper
- for a bond below the plane of the paper
- for a bond above the plane of the paper

Using this symbolism, the structural formulas shown above can be redrawn in the following fashion.
In this experiment, you will construct three-dimensional models to help you visualize the shapes of molecules. You will use ball-and-stick type models, in which colored plastic balls represent atoms and short plastic connectors represent the bonds. Double and triple bonds are represented by thin flexible connectors and thick inflexible connectors serve as single bonds. The plastic balls have holes molded into them to accept the connectors. The number of holes in the ball represents the maximum number of bonds that a given atom can have. The balls are color-coded so that atoms of different elements can be distinguished. A typical system is shown in the table below.

<table>
<thead>
<tr>
<th>Atom</th>
<th>Symbol</th>
<th>Color</th>
<th>Number of Holes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H</td>
<td>White</td>
<td>1</td>
</tr>
<tr>
<td>Carbon</td>
<td>C</td>
<td>Black</td>
<td>4</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O</td>
<td>Red</td>
<td>2</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N</td>
<td>Blue</td>
<td>3</td>
</tr>
<tr>
<td>Chlorine (Halogens)</td>
<td>Cl</td>
<td>Green</td>
<td>1</td>
</tr>
<tr>
<td>Sulfur</td>
<td>S</td>
<td>Yellow</td>
<td>2 or 6</td>
</tr>
</tbody>
</table>

**VSEPR Theory**

In reality, molecules exist in three dimensions. The Valence-Shell Electron-Pair Repulsion theory, or VSEPR theory, explains and predicts these three dimensional shapes. The theory states that *because electron pairs repel* (both have negative charge), molecules adjust their shapes so that the valence-electron pairs are as far apart as possible. There are several basic shapes that are then developed by small molecules (no more than several atoms) and these basic shapes are shown below. As you build the molecules in this lab activity, you may refer to these diagrams to assist you in identifying the shape of each molecule made.
<table>
<thead>
<tr>
<th>Name</th>
<th>Formula</th>
<th>Structural representation</th>
<th>Shape (name)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) hydrogen (molecular)</td>
<td>H₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2) water</td>
<td>H₂O</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3) methane</td>
<td>CH₄</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4) chlorine (molecular)</td>
<td>Cl₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5) ammonia</td>
<td>NH₃</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6) nitrogen (molecular)</td>
<td>N₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7) ethyne</td>
<td>C₂H₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8) phosphorus pentachloride</td>
<td>PCl₅</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
9) dichloromethane \( \text{CH}_2\text{Cl}_2 \)

10) 1-propanol \( \text{C}_3\text{H}_7\text{OH} \)

11) carbon dioxide \( \text{CO}_2 \)

12) methanol \( \text{CH}_3\text{OH} \) This molecule is more complex than the basic shapes shown in these lab instructions

13) hydrogen peroxide \( \text{H}_2\text{O}_2 \)

14) oxygen (molecular) \( \text{O}_2 \)

15) hydrogen sulfide \( \text{H}_2\text{S} \)
<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>16) ethene</td>
<td>$\text{C}_2\text{H}_4$</td>
<td>This molecule is more complex than the basic shapes shown in these lab instructions</td>
</tr>
<tr>
<td>17) propane</td>
<td>$\text{C}_3\text{H}_8$</td>
<td>This molecule is more complex than the basic shapes shown in these lab instructions</td>
</tr>
<tr>
<td>18) propene</td>
<td>$\text{C}_3\text{H}_4$</td>
<td>This molecule is more complex than the basic shapes shown in these lab instructions</td>
</tr>
<tr>
<td>19) ethanol</td>
<td>$\text{C}_2\text{H}_5\text{OH}$</td>
<td>This molecule is more complex than the basic shapes shown in these lab instructions</td>
</tr>
<tr>
<td>20) methylamine</td>
<td>$\text{CH}_3\text{NH}_2$</td>
<td>This molecule is more complex than the basic shapes shown in these lab instructions</td>
</tr>
<tr>
<td>21) sulfur hexafluoride</td>
<td>$\text{SF}_6$</td>
<td></td>
</tr>
<tr>
<td>22) ethanoic acid</td>
<td>$\text{CH}_3\text{COOH}$</td>
<td>This molecule is more complex than the basic shapes shown in these lab instructions</td>
</tr>
</tbody>
</table>
23) Construct a model of butane, $\text{C}_4\text{H}_{10}$. Draw a sketch of this molecule. Can you construct a model of a different molecule having the same molecular formula as butane? **Structural isomers** are two or more chemical compounds with the same chemical formulae but different structural formulae or different spatial arrangements of atoms. The different forms are known as **isomers**. This type of structural isomer differs in the location of a functional group. The functional group that is switched around in this molecule is a $-\text{CH}_3$ called a “methyl group.”

![Diagram of n-butane and iso-butane](image)

24) Another type of structural isomer results in compounds with different types of functional groups. Construct a model of ethanol, $\text{C}_2\text{H}_5\text{OH}$ (see number 19 in this lab). Then, construct a model of dimethyl ether, $\text{CH}_3\text{OCH}_3$. Draw them each below and compare the number of carbons, hydrogens, and oxygens in each.

![Diagram of ethanol and dimethyl ether](image)

Number of C=_______; H=_______; O=_______

Number of C=_______; H=_______; O=_______

These isomers have different physical and chemical properties. Structural isomers play a very important role in organic chemistry.
**Stereoisomerism (Two Types)**

**Optical Isomerism:** Construct a model of bromochlorofluoromethane, CHBrClF. Use a different color ball for each halogen. Sketch the compound. Construct an isomer of this compound keeping carbon at the center (a different arrangement of the same atoms)? Hint: Is your left hand identical to your right? Keeping your first model, make another one that matches it.

25) bromochlorofluoromethane CHBrClF

Draw both sets of structures

These two compounds have the same molecular formula, CHBrClF, but they are different from each other in the way that a left hand is different from a right hand. The compounds are mirror-images of each other and have no plane of symmetry. They are also called chiral molecules – having a central carbon attached to four different groups. The phenomenon of “handedness” is especially important in biochemistry.

**Cis-trans isomerism** is another type of stereoisomerism. This occurs when there is restricted rotation about a bond between two atoms. Groups attached to each atom may be on the same side of the bond (the cis isomer) or opposite sides (the trans isomer). Cis-trans isomerism also occurs in some inorganic complex compounds, when two groups may be at adjacent (cis) or opposite (trans) positions.

26) Construct a model of cis-1,2-dichloroethane and another model of trans-1,2-dichloroethane. Both molecules have the formula C₂H₂Cl₂.

HINT: the carbons are bonded to each other, and each carbon is bonded to one hydrogen and one chlorine.

Draw both structures