MOLECULAR MODEL BUILDING

Background
Models help us visualize the structures of atoms and molecules that are too small to see. The relationship between the location of an element in the Periodic Table and the set of chemical and physical properties that element exhibits is due to the periodic (repeating) nature of atomic structure. Most of the observable chemical and physical properties of the elements can be accounted for by the arrangement of the electrons in each element. The arrangement of electrons of the elements in a chemical family (vertical column) is very similar, giving rise to a fundamental relationship between structure and function – elements with similar electron configurations exhibit similar properties, one of those being the tendency to form the same number of bonds in chemical compounds. The electrons that are involved in bond formation are those farthest from the nucleus, the valence electrons.

The shapes of covalent compounds (atoms held together in a molecule by covalent bonds) can be specified by giving the internuclear distances and the angle between two bonds. This information can be determined experimentally using X-ray crystallographic techniques. To display the shapes of molecules, several representations can be drawn, or models can be constructed from a variety of materials. Bonds are typically represented as sticks or springs, atoms as balls of different colors, to represent various elements. Computer programs have also been developed to display three-dimensional representations of molecules based on ball and stick representations, or space-filling representations (for which the location and length of bonds is less clear).

For more information: see chapters 2 and 3 in Chemistry in Context, and for a more in depth treatment of this topic see General Chemistry by Jean Umland (first edition available for loan in the stockroom).

Procedure
In this experiment, you will construct models for several assigned molecules. You will then be asked to build the model for an unfamiliar molecule. As you build your molecules, you may visit several World Wide Web Sites (which will be provided for you) to view the structures for your molecules or similar molecules. You will be asked to draw the ball and stick representations for the models you build, and for several molecules whose 3-D structures you will view on the Web.

Building Models
The Model Building Kits are available in the stockroom (room 141). Atoms are represented by balls of different colors, single bonds by sticks, and multiple bonds by springs. This particular kit does not have a specific means for indicating lone pairs, but a wooden stick (single bond stick) with no atom attached to one end can serve as a reminder that there is a lone pair on an atom. Atoms of the elements are represented by the colors shown at right:

<table>
<thead>
<tr>
<th>Color</th>
<th>Element</th>
</tr>
</thead>
<tbody>
<tr>
<td>Black</td>
<td>Carbon</td>
</tr>
<tr>
<td>Blue</td>
<td>Nitrogen</td>
</tr>
<tr>
<td>Yellow</td>
<td>Hydrogen</td>
</tr>
<tr>
<td>Red</td>
<td>Oxygen</td>
</tr>
<tr>
<td>Green</td>
<td>Chlorine</td>
</tr>
<tr>
<td>Orange</td>
<td>Bromine</td>
</tr>
<tr>
<td>Purple</td>
<td>Iodine</td>
</tr>
</tbody>
</table>

We will be discussing molecular structure in terms of the shapes described by atoms linked by covalent bonds (single or multiple). The set of guidelines that we will use to assist us are taken from one description of molecular bonding called Valence Shell Electron Pair Repulsion Theory (or VSEPR for short). VSEPR is very useful for predicting molecular shapes for simpler molecules. (For more complex molecules, Molecular Orbital Theory gives a more thorough treatment, and is found in General Chemistry by Umland, for those with the interest or need to pursue this topic in more detail). The rules for drawing Lewis Dot Structures are the same as those found in your text book, and are also derived from VSEPR theory.

Keep in mind that part of this Theory of molecular structure is the octet rule, which states that atoms have a tendency to form bonds until each atom has, through sharing or lone pairs, eight electrons in the
valence shell. Indeed, the driving force for atoms to forms bonds is to achieve a stable arrangement of electrons in the valence shell. The most stable arrangement of electrons is that observed for the Noble Gases, which have eight electrons in the outer shell. This is the basis for the octet rule, and most atoms obey this rule when forming bonds.

There are several noteworthy exceptions: Hydrogen is a very small atom, and forms only one bond, for a maximum of 2 electrons in the valence shell. Beryllium forms 2 bonds and boron forms 3 bonds. These small atoms form stable compounds with fewer than eight electrons in the valence shell (BeCl₂ and BF₃ are the classic examples).

**Rules for Drawing Lewis Dot Structures and Predicting Molecular Shapes Using VSEPR**

1. Correctly identify the formula of the molecule under discussion.

2. Using the Periodic Table, calculate the total number of valence electrons available for the molecule. For CCl₄, the total number of valence electrons:

   1 C atom per molecule x 4 valence electrons = 4
   4 Cl atoms per molecule x 7 valence electrons = 28

   total = 32 valence electrons

3. Choose a central atom or atoms. This is generally the atom of lowest electronegativity. For CCl₄, the central atom is Carbon. Electronegativity may be estimated from relative position on the Periodic Table, or you may use numerical values given in Chapter 5 of *Chemistry in Context*.

For many simple molecules, the formula may also give you some information about the central atom: for formulas in the form ABₓ, indicating one atom of A and two or more of B, then element A is the central atom.

For organic compounds with two or more carbons, the carbons are typically found bonded to each other in a central chain, or “backbone”, with hydrogens or other groups attached to individual carbons. Formulas and systematic names for complex molecules also provide more structural information.

**Examples:**

\[ \text{BF}_3 \]
central atom B
24 total valence electrons

\[ \text{C}_3\text{H}_6 \]
C-C-C chain in molecule
20 total valence electrons

4. Draw the central atom (symbol for the element as indicated in the formula), then draw the symbols for the other elements around it, as far from each other as possible.

For CCl₄:

\[
\begin{array}{ccc}
\text{Cl} & \text{Cl} & \text{Cl} \\
\text{Cl} & \text{C} & \text{Cl} \\
\text{Cl} & \text{F} & \text{F} \\
\end{array}
\]

For BF₃:

\[
\begin{array}{ccc}
\text{F} & \text{F} & \\
\text{B} & \text{H} & \text{C} \\
\text{H} & \text{C} & \text{C} & \text{H} \\
\end{array}
\]

For C₃H₆:

\[
\begin{array}{ccc}
\text{H} & \text{H} & \text{H} \\
\text{H} & \text{C} & \text{C} \\
\text{H} & \text{H} & \text{H} \\
\end{array}
\]

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5. Draw a line (or two dots) to represent a covalent bond between the central atom and each surrounding atom. Keep track of how many valence electrons you have used.

For \( \text{CCl}_4 \):  
\[ \begin{array}{c}
\text{Cl} \\
\text{Cl} \\
\text{Cl} \\
\text{Cl}
\end{array} \]

For \( \text{BF}_3 \):  
\[ \begin{array}{c}
\text{F} \\
\text{B} \\
\text{F}
\end{array} \]

For \( \text{C}_3\text{H}_8 \):  
\[ \begin{array}{c}
\text{H} \\
\text{H} \\
\text{H} \\
\text{H} \\
\text{H} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{H}
\end{array} \]

Valence Electrons remaining to be placed:

For \( \text{CCl}_4 \): 24  
For \( \text{BF}_3 \): 18  
For \( \text{C}_3\text{H}_8 \): zero electrons to place - structure complete  
(Remember: Hydrogen only forms one bond, and has no more than two electrons in its outer shell (no lone pairs).

6. Use the remaining valence electrons to complete the valence octet for each outer atom. Do this by placing pairs of non-bonded electrons (lone pairs) around the outer atoms.

For \( \text{CCl}_4 \):  
\[ \begin{array}{c}
\text{Cl} \\
\text{Cl} \\
\text{Cl} \\
\text{Cl}
\end{array} \]

For \( \text{BF}_3 \):  
\[ \begin{array}{c}
\text{F} \\
\text{B} \\
\text{F}
\end{array} \]

These structures are now complete. The central atom and each attached atom have complete octets, and all valence electrons have been placed in bonds or lone pairs.

7. With any remaining valence electrons, complete the octet around the central atom with lone pairs (if needed).

8. If the octets of all (non-hydrogen) atoms cannot be completed with lone pairs, then multiple bonds are necessary. Two pairs of electrons shared between two atoms form a double bond, three shared pairs form a triple bond. The electrons in shared pairs are counted for each atom.

When you have completed the assigned molecules, you will be given another compound by your Lab Instructor. You will analyze this compound as before, and present your assigned compound to the class, showing the model and describing how you arrived at the structure for your compound. This presentation will be worth 10% of the grade for this lab.

On the Web

Look for two molecules that will be given to you by your Instructor, at the World Wide Web sites provided for you. Draw the Lewis structures for these and answer the assigned questions.

Procedure

1. Draw the Lewis Structure for each compound, along with any resonance structures.

2. Determine if any structural isomers exist.
3. Construct a model for the compound, one for each isomer. Remember the models will not show the position of the lone pairs.

4. Use the list of examples to assign structural geometry to your compounds, as defined by the position of the bonds and atoms.

**Examples of Molecular Shape**

<table>
<thead>
<tr>
<th>Arrangement of Electron Pairs Around the Central Atom</th>
<th>Molecular Shape</th>
<th>Approximate Angle Between Bonded Pairs</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 pairs, single bonded</td>
<td>tetrahedral</td>
<td>109.5</td>
</tr>
<tr>
<td>3 pairs, single bonded</td>
<td>trigonal pyramid</td>
<td>107.5</td>
</tr>
<tr>
<td>1 lone pair</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 pairs, single bonded</td>
<td>bent</td>
<td>104.5</td>
</tr>
<tr>
<td>2 lone pairs</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 pair single bonded, 3 lone pairs</td>
<td>not a central atom</td>
<td></td>
</tr>
<tr>
<td>1 double bond (2 pair)</td>
<td>planar triangular</td>
<td>120</td>
</tr>
<tr>
<td>2 pairs, single bonded</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 double bonds (4 pairs)</td>
<td>linear</td>
<td>180</td>
</tr>
</tbody>
</table>

5. Decide whether the molecule is polar or nonpolar. Remember: molecules with polar bonds can still be nonpolar molecules!
<table>
<thead>
<tr>
<th>Compound</th>
<th>Total Valence Electrons</th>
<th>Lewis Structure</th>
<th>Molecular Shape</th>
<th>Polar Bonds?</th>
<th>Polar Molecule?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br₂</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>CH₄</td>
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<td></td>
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<tr>
<td>NH₃</td>
<td></td>
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<tr>
<td>H₂O</td>
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</tr>
<tr>
<td>CCl₄</td>
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<tr>
<td>CO₂</td>
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<td></td>
</tr>
<tr>
<td>Compound</td>
<td>Total Valence Electrons</td>
<td>Lewis Structure</td>
<td>Molecular Shape</td>
<td>Approximate Bond Angle</td>
<td>Polar Bonds?</td>
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<tr>
<td>$O_2$</td>
<td></td>
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<tr>
<td>$O_3$</td>
<td></td>
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</tr>
<tr>
<td>$NO_2$</td>
<td></td>
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<tr>
<td>$CF_2Cl_2$</td>
<td></td>
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</tr>
<tr>
<td>$C_2H_6O$</td>
<td></td>
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<td></td>
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<tr>
<td>assigned compound (see Lab Instructor)</td>
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</tr>
<tr>
<td>Compound</td>
<td>Total Valence Electrons</td>
<td>Lewis Structure</td>
<td>Molecular Shape</td>
<td>Approximate Bond Angle</td>
<td>Polar Bonds?</td>
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