# Molecular Models: A Study Assignment

#### **Performance Goals**

- **15–1** Write Lewis (electron dot) diagrams for molecules and ions formed by representative elements.
- **15–2** Predict the polarity of bonds and molecules formed by representative elements.
- **15–3** Predict bond angles and shapes of molecules and polyatomic ions.
- 15–4 Construct models for some covalently bonded species.

#### CHEMICAL OVERVIEW

Chemical bonds are the forces that hold atoms together in a compound. In this experiment we will study only covalently bonded species. A covalent bond is formed when a pair of electrons is shared by two atoms. Bonds in which the electrons are shared equally by the two nuclei are described as **nonpolar**. We expect to find nonpolar bonds whenever two identical atoms are joined, such as H<sub>2</sub> or Cl<sub>2</sub>.

When different atoms are joined, the polarity of the bond depends on the electronegativity difference between the two elements. In the HF molecule, for example, the electron density is greater around the fluorine atom and the bond has a nonsymmetrical or nonuniform electron distribution. This type of a bond is referred to as **polar**.

We find experimentally that bonds formed between atoms that differ in electronegativity by 0.4 unit or less (such as the C—H bond) behave very much like pure nonpolar bonds and therefore may be classified as "essentially nonpolar." Bonds with an electronegativity difference greater than 1.7 are regarded as **ionic** bonds. (HF is an exception.) Electronegativity values for some common elements are listed in Table 15.1.

When determining whether a *molecule* is polar or not, its structure as well as the type of bonds in the molecule must be considered. If the molecule *has* at least one polar bond *and* is *nonsymmetrical*, it will be polar. On the other hand, even if the molecule has polar bonds, but is structurally symmetrical, the species will be nonpolar.<sup>\*</sup> Obviously, if there are no polar bonds in a molecule, it will be nonpolar.

<sup>\*</sup>The question of polarity does not apply to ionic species since they carry an overall charge.

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Element	Electroneg.	Element	Electroneg.
Н	2.1	Si	1.8
В	2.0	Р	2.1
С	2.5	S	2.5
Ν	3.0	Cl	3.0
О	3.5	Br	2.8
F	4.0	Ι	2.5

 Table 15.1
 Selected Electronegativity Values

In this experiment you will be asked to determine the polarity of certain bonds and, after considering the geometry of the molecule, decide whether it is polar or nonpolar.

#### Lewis (Electron Dot) Diagrams

In most stable molecules or polyatomic ions, each atom tends to acquire a noble-gas structure by sharing electrons. This tendency is often referred to as the **octet rule**. One way to show the structure of an atom or a molecule is by using dots to represent the outermost *s* and *p* electrons (the so-called **valence electrons**). For the A group elements the number of valence electrons is the same as the group number in the periodic table.

Group	IA	IIA	IIIA	IVA	VA	VIA	VIIA	0
No. of valence electrons	1	2	3	4	5	6	7	8
Lewis structure	Li•	Be	:ġ	:Ċ·	÷Ņ∙	÷ö∙	:Ë·	:Ne:

In writing Lewis diagrams we usually do not attempt to show which atom the valence electrons come from; we simply indicate a shared pair of electrons by either two dots or a straight line connecting the atoms. Unshared pairs, also called lone pairs, are indicated by dots written around the elemental symbols. Example:

$$H_2O$$
  $H$   $H$   $NH_3$   $H$   $H$ 

Atoms in polyatomic ions are held together by covalent bonds. In the ions we will consider in this assignment, all atoms have a noble-gas structure.

Occasionally, too few electrons are available in a species to allow an octet to exist around each atom with only single bonds. In these instances multiple (double or triple) bonds will form.

Writing Lewis Structures
The Lewis diagrams of many species can be drawn by inspection. For more complex species, however, the following procedure is helpful:
1. Draw a tentative diagram for the molecule or ion, joining atoms by single bonds. Place electron dots around each symbol except hydrogen so the total number of electrons for each atom is eight. In some cases, only one arrangement of atoms is possible. In others, two or more structures may be drawn. Ultimately chemical or physical evidence must be used to decide which of the possible structures is correct. A few general rules will help you in drawing diagrams that are most likely to be correct:
a. A hydrogen atom always forms one bond; a carbon atom normally

forms four bonds.

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- **b.** When several carbon atoms appear in the same molecule, they are often bonded to each other. In some compounds they are arranged in a closed loop; however, we will avoid such so-called cyclic compounds in this assignment.
- **c.** In compounds or ions having two or more oxygen atoms and one atom of another nonmetal, the oxygen atoms are usually arranged *around* the central nonmetal atom.
- **d.** In an oxyacid (hydrogen + oxygen + a nonmetal, such as  $H_2SO_4$  or  $HNO_3$ ), hydrogen is usually bonded to an oxygen atom, which is then bonded to the nonmetal:  $H\_O\_X$ , where *X* is a nonmetal.
- 2. Count the electrons in your diagram.
- **3.** Find the total number of valence electrons available. For a molecule, this is the sum of the valence electrons contributed by each atom in the molecule. For a polyatomic ion, this total must be adjusted to account for the charge on the ion. An ion with a -1 charge will have one more electron than the number of valence electrons in the neutral atoms; a -2 ion, two more; a +1 ion, one less; and so forth.
- 4. Compare the numbers in Steps 2 and 3. If they are the same, the diagram is complete. If they are different, modify the diagram with multiple bonds. If your diagram has two electrons more than the number available, there will be one double bond. If the difference is four, there will be a triple bond or two double bonds. Multiple bonds should be used only when necessary, and then as few as possible should be used.
- 5. The most common elements that can form a double bond are C, N, O, Si, P, and S.
- 6. The most common elements that can form a triple bond are C, N, Si, and P.
- 7. Halogens (i.e., Cl, Br, I) only form single bonds unless they are the center atom.

There are some exceptions to the octet rule. It is not possible to write a Lewis diagram that has eight electrons around each atom if the total number of valence electrons is odd. Also, for compounds of Group IA, IIA, and IIIA elements, there are not enough electrons to satisfy the octet rule.

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**Electron Pair and Molecular Geometry** Several theories are used to explain the geometry (three-dimensional shape) of molecules. In this experiment we will use the valence shell electron pair repulsion (VSEPR) theory. According to this theory, electrostatic repulsion arranges the electron pairs surrounding an atom so that they are as far from each other as possible. This arrangement is the **electron pair geometry**. The molecular geometry, the arrangement of *atoms* around the central atom, is a direct result of the electron pair geometry.

Let us consider cases in which the central atom is surrounded by 2, 3, or 4 electron pairs.

- **1. Two pairs of electrons**. Two pairs of electrons around a central atom are farthest from each other when they are on opposite sides of that atom. The electron pairs and the central atom are on the same straight line. The electron pair geometry is **linear**. Both electron pairs bond atoms to the central atom, so all three atoms are also on the same line. The molecular geometry is linear too.
- **2.** Three pairs of electrons. Three electron pairs will be farthest apart when they are directed toward the corners of an equilateral triangle with the central atom at its center. The atom and all electron pairs are in the same plane, so the electron pair geometry is called **trigonal planar**, or **planar triangular**. If all three electron pairs are bonding pairs, the molecule is also planar triangular, with 120° bond angles. If one of the electron pairs is a lone pair, the molecular geometry is **bent** or **angular**.
- **3.** Four pairs of electrons. Four pairs of electrons in three dimensions are farthest apart when located at the corners of a tetrahedron with the central atom in its center. If all four electron pairs are bonding pairs, as in CH<sub>4</sub>, the central carbon atom is in the center of the tetrahedron and the four hydrogen atoms are at its corners. Both the electron pair and molecular geometries are **tetrahedral**. The bond angles are 109°.

If there are three bonding pairs and one lone pair, as in the NH<sub>3</sub> molecule, VSEPR still predicts a tetrahedral electron pair geometry with a tetrahedral angle for the bonding electron pairs. (In fact, the angle is slightly less than tetrahedral, but we will call it a "tetrahedral" angle.) The molecule has the shape of a low pyramid; its geometry is **trigonal pyramidal**. Two bonding pairs and two lone pairs around the central atom again yield close to a tetrahedral angle. The three-atom molecule has a **bent** geometry.

These electron pair and molecular geometries are summarized in Table 15.2.

#### Multiple Bonds

Bond angles in species that contain multiple bonds indicate that the electrons in the multiple bond behave as a single pair of electrons according to VSEPR. Thus a structure such as



has a planar triangular geometry around the C atom with  $120^\circ$  bond angles.

Total No. Electron Pairs	Shared	Unshared	Bond Angle	Electron Pair Geometry	Molecular Geometry	Example
2	2	0	$180^{\circ}$	Linear	Linear	BeF <sub>2</sub>
3	3	0	$120^{\circ}$	Trig. planar	Trig. planar	BF <sub>3</sub>
3	2	1	$120^{\circ}$	Trig. planar	Angular (bent)	$NO_2^-$
4	4	0	$109^{\circ}$	Tetrahedral	Tetrahedral	$CCl_4$
4	3	1	$109^{\circ}$	Tetrahedral	Trigonal pyramidal	$\mathrm{NH}_3$
4	2	2	$109^{\circ}$	Tetrahedral	Bent	H <sub>2</sub> O

Table 15.2         Electron Pair and Molecular Geome
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#### PROCEDURE

Obtain a molecular model kit. Draw a Lewis diagram for HCl, the first item in the table on the work page. From your diagram, and using Table 15.2 as a guide, fill in all the blanks for HCl. Then build a model of an HCl molecule. Use the model to verify the geometry you predicted. If the model and your prediction do not agree, find out why. Do not proceed to  $H_2O$  until you thoroughly understand the HCl structure.

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Follow the same procedure with  $H_2O$ , the next item in the table. This time you must predict a bond angle too. Your model should confirm your predictions. Again, do not proceed to  $NH_3$  until you thoroughly understand  $H_2O$ .

Proceed in a similar manner for all species shown in the table. From a learning standpoint, it is important that you complete each species, including the model, before you proceed to the next.

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## **Experiment 15**

**Advance Study Assignment** 

**1.** Define electron pair and molecular geometry. When are these the same and when are they different? Give an example.

**2.** Draw Lewis structures for  $CO_2$ ,  $SO_2$ , and  $NO_3^-$ .

**3.** Give the electron pair geometry and the molecular geometry of the three species from Question 2, according to VSEPR.

4. Are CO<sub>2</sub> and SO<sub>2</sub> polar or nonpolar molecules? Explain your reasoning.

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### **Experiment 15**

Work Page

Instructions: For each species listed below, draw the Lewis structure first and then complete the rest of the information requested for that species. "Build" the molecule or ion with your model kit. Verify from your model the geometry you predicted. Fill out each line and build the model before proceeding to the next line. If there are more than two atoms as "center," you can only deduce the geometry separately for each one. Continue this procedure for each species listed here.

Nonpolar						×	×
Polar						×	×
Bond Angle	×						
Molecular Geometry							
Electron Pair Geometry	×						
Lewis Structure							
Formula	НСІ	$H_2O$	$\mathrm{NH}_3$	BCl <sub>3</sub>	CO <sub>2</sub>	$\mathrm{IO_2}^-$	$\mathrm{PO_4^{3-}}$

Formula	Lewis Structure	Electron Pair Geometry	Molecular Geometry	Bond Angle	Polar	Nonpolar
$C_2H_6$						
$C_2H_4$						
$C_2H_2$		Around O	Around O			
C <sub>2</sub> H <sub>5</sub> OH						
НСНО		Around O	Around O			
CH <sub>3</sub> —O—CH <sub>3</sub>		Around C	Around C			
НСООН		Around single-bonded O	le-bonded O			
CH <sub>3</sub> COOH						

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### **Experiment 15**

### **Report Sheet**

Instructions: For each species listed below, draw the Lewis structure first and then complete the rest of the information requested for that species. "Build" the molecule or ion with your model kit. Verify from your model the geometry you predicted. Fill out each line and build the model before proceeding to the next line. If there are more than two atoms as "center," you can only deduce the geometry separately for each one. Continue this procedure for each species listed here.

Nonpolar						×	×
Polar						X	×
Bond Angle	×						
Molecular Geometry							
Electron Pair Geometry	×						
Lewis Structure							
Formula	HCI	$H_2O$	°HN	BCI <sub>3</sub>	CO <sub>2</sub>	$\mathrm{IO}_2^-$	$\mathrm{PO_4^{3-}}$

Formula	Lewis Structure	Electron Pair Geometry	Molecular Geometry	Bond Angle	Polar	Nonpolar
C <sub>2</sub> H <sub>5</sub> OH		Around O	Around O			
CH <sub>3</sub> —0—CH <sub>3</sub>		Around O	Around O			
НСООН		Around C	Around C			
СН <sub>3</sub> СООН		Around single-bonded O	le-bonded O			

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