STUDENT

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Lewis Structures and Molecular Geometry

Student Laboratory Kit

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Introduction

Molecules have shape! The structure and shape of a molecule influences its physical properties and affects its chemical behavior as well. Lewis structures and VSEPR theory offer useful models for visualizing the structures of covalent compounds.

Concepts

- Valence electrons
- Lewis structures
- Covalent bonding
- VSEPR theory

Background

Covalent bonds are defined as the net attractive forces between nonmetal atoms that share one, two, or three pairs of electrons. In general, only the *valence electrons,* those in the highest energy levels that are farthest away from the nucleus, are available for bonding. The number of valence electrons influences the number of bonds that an atom will form. The periodic table offers a convenient shortcut for determining the number of valence electrons in an atom. Remember that the position of an element in the modern periodic table reflects its electron configuration. When the representative elements are arranged in columns from IA to VIIIA (Figure 1), the number of valence electrons for an element is equal to its group number. Thus, potassium in Group IA has one valence electron, carbon in Group IVA has four valence electrons, and chlorine in Group VIIA has seven valence electrons. In 1916, G. N. Lewis, an American chemist, proposed arranging dots around the symbols of the elements to represent the valence electrons. *Lewis electron-dot symbols* (Figure 2 on page 2) remain the most popular way to illustrate the valence electrons that are available for bonding.

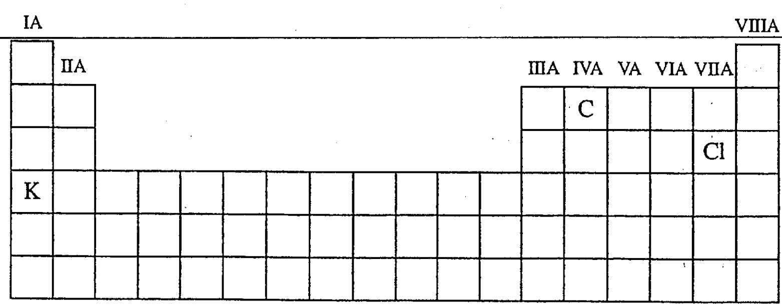


Figure 1. Numbering of Representative Elements in Groups IA–VIIIA.

K·   ·C̈· (with a dot below)   :C̈l·

Figure 2. Lewis Electron-Dot Symbols for Representative Elements.

Lewis structures build on the Lewis electron-dot symbols of the elements to show the bonding arrangement of atoms in a molecule and the distribution of all valence electrons. The Lewis structure of a molecule thus shows all of the atoms and how they are connected. A single covalent bond between two atoms, corresponding to a pair of electrons, is represented using a dash (—). Sometimes atoms share more than one pair of electrons between them in order to form stable molecules. Two dashes, corresponding to two pairs of electrons, and three dashes, corresponding to three pairs of electrons, are used to represent double and triple bonds, respectively.

G. N. Lewis offered a simple theory, based on the known stability of the noble gases (He, Ne, etc.), to predict how many bonds an atom will form and how many atoms of a particular type will come together to form a stable molecule. According to Lewis, nonmetals may share electrons in order to achieve a valence shell electron "count" similar to that of the noble gases:

> *"Two atoms may conform to the rule of eight, or the octet rule . . . by sharing one or more pairs of electrons. The electrons which are held in common by two atoms may be considered to belong to the outer shell of both atoms."*

The noble gases have filled s and p orbitals with eight electrons. The octet rule assumes that atoms form molecules to achieve this stable, noble gas electron configuration. In counting valence electrons to predict the structure of a covalent compound, we will distinguish between two kinds of electron pairs. Bonding pairs of electrons are shared between atoms and thus "belong" to both atoms in the bond. Nonbonding or unshared pairs of electrons are not shared between atoms and are therefore "counted" toward only one of the atoms. Consider the fluorine molecule (F_2). Each fluorine atom has seven valence electrons and needs only one more electron to form a stable molecule—two fluorine atoms come together and share one bonding pair of electrons (Equation 1). Each fluorine atom retains its three unshared pairs of electrons.

$$:\ddot{\underset{\cdot\cdot}{F}}\cdot \;+\; \cdot\ddot{\underset{\cdot\cdot}{F}}: \;\longrightarrow\; :\ddot{\underset{\cdot\cdot}{F}}:\ddot{\underset{\cdot\cdot}{F}}: \qquad \text{Equation 1}$$

$$:\ddot{\underset{\cdot\cdot}{F}}-\ddot{\underset{\cdot\cdot}{F}}:$$

Lewis Structure of Fluorine

Molecular Geometry

According to the *Valence Shell Electron Pair Repulsion* (VSEPR) theory, the valence electron pairs that surround an atom repel each other due to their like negative charges. In order to minimize this repulsion, the electron pairs should be positioned around the atom so that they are as far apart as possible. The resulting symmetrical arrangement of electron pairs around atoms can be used to predict molecular geometry—the three-dimensional shape of a molecule. Two pairs of electrons around an atom should adopt a linear arrangement, three pairs a trigonal planar arrangement, and so on.

The three-dimensional structure of a molecule is affected by the spatial arrangement of *all* the electron pairs—both bonding and nonbonding—around the central atom. However, only the physical arrangement of the *atoms* is used to describe the resulting molecular geometry. This is best illustrated using an example. The Lewis structure of the water molecule is shown as the first example in Figure 3—there are four pairs of valence electrons around the central oxygen atom. Two pairs of electrons are involved in bonding to hydrogen atoms, while the other two electron pairs are unshared pairs. Four pairs of electrons around an atom will adopt a tetrahedral arrangement in space, as depicted in the second example in Figure 3, to be as far apart in space as possible. For this representation, the symbol " ıııııııı····· " shows one lone pair of electrons extending behind the plane of the paper. The symbol " ◀▬▬ " shows one lone pair of electrons extending in front of the plane of the paper, while the symbols "——" represent the hydrogen–oxygen bonds positioned in the plane of the paper. As a result, the two hydrogen atoms and the oxygen atom occupy a "bent" (inverted-V) arrangement.

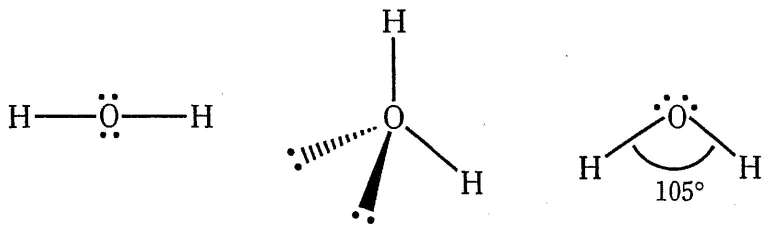


Figure 3. Lewis Structure of Water and Its Molecular Geometry.

When two atoms are linked via a double or triple bond (with two or three bonding pairs of electrons, respectively), the multiple electron pairs between the atoms must be considered together when determining the shape of the molecule. Carbon dioxide provides a good example (Figure 4). The central carbon atom is linked to two oxygen atoms by two double bonds. The resulting arrangement of atoms is linear—both electron pairs in each double bond are considered to be one electron group that must be in approximately the same region, near the oxygen atom.

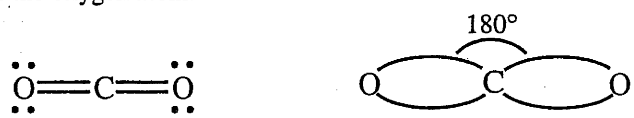


Figure 4. Lewis Structure of Carbon Dioxide and Its Molecular Geometry.

Experiment Overview

The purpose of this activity is to practice drawing Lewis structures of molecules and to use these structures to predict their molecular geometry. Molecular models will be studied to visualize the shapes of molecules and to sketch their three-dimensional structures.

Pre-Lab Questions

1. Write the Lewis electron-dot symbol for each of the following atoms: hydrogen, boron, nitrogen, silicon, sulfur, and bromine.
2. What information about a molecule does its Lewis structure provide? What information is neither shown nor implied in the Lewis structure?
3. There are several exceptions to the octet rule.
   a. Based on its electron configuration, explain why hydrogen can only have two valence electrons around it when it bonds to other atoms. What is the maximum number of bonds hydrogen will form?
   b. Neutral compounds of boron may be described as "electron-deficient." Based on its electron configuration, predict how many covalent bonds boron will form. Is this the maximum number of bonds boron will form? *Hint:* Boron forms polyatomic ions.
   c. Many elements in the third row and beyond in the periodic table may form more than four bonds and thus appear to have "expanded octets." Phosphorus and sulfur, for example, may form five and six covalent bonds, respectively. Count up the total number of valence electrons in PCl_5 and draw its Lewis structure. How many valence electrons are "counted" toward the central P atom?

Materials

Periodic table

Set of molecular models labeled A through K

Safety Precautions

Although this activity is considered nonhazardous, observe all normal laboratory safety guidelines.

Procedure

Part A. Lewis Structures

1. Write the formula for each molecule or polyatomic ion listed in Data Table A. Some of the formulas have been filled in for you.

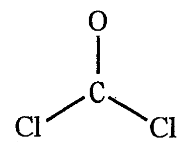
2. Count the number of valence electrons supplied by each atom in the formula. Determine the *total number* of valence electrons and record this number in Data Table A. In the case of polyatomic ions, *add* one electron for each unit of *negative* charge or *subtract* one electron for each unit of *positive* charge to determine the total number of valence electrons.

3. Use the following guidelines to draw a reasonable Lewis structure for each molecule or ion in the space provided. If more than one Lewis structure is reasonable, draw all of the appropriate Lewis structures. *Note:* Keep in mind the exceptions to the octet rule discussed in the *Pre-Lab Questions*.

- Draw a "skeleton" structure for the molecule or ion, joining atoms by single bonds. If there is a single atom of one element in a compound, show it as the *central atom* with other atoms joined to it. The least electronegative atom is usually the central atom. However, hydrogen is never a central atom.
- From the total number of valence electrons, subtract two for each single bond in the skeleton—this tells you how many valence electrons are left to distribute.
- Use the octet rule to distribute the remaining valence electrons as unshared pairs around the atoms in the molecule or ion.
- If this point is reached and there are too few valence electrons to give each atom an octet, multiple bond(s) may be needed. Remember that bonding electrons are "counted" toward both atoms in the bond, while unshared electrons are "assigned" to only one atom.

Example:

$COCl_2$ has 24 valence electrons.



$24 - (3 \times 2) =$ 18 valence electrons must be distributed.

- If all else fails, some Lewis structures can only be drawn by assuming there is an unpaired electron in the molecule.

Part B. Molecular Models

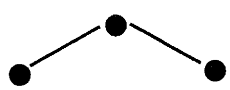
4. Examine the molecular models A–K. For each model, identify the number of bonding pairs, the number of unshared pairs, and the total number of electron pairs around the *central atom*. Record this information in Data Table B. *Note:* In the case of double or triple bonds, count all of the electrons involved in the bond as *one pair* of electrons. (Review the structure of carbon dioxide in the *Background* section.)

5. Sketch the three-dimensional arrangement of valence electron pairs around each central atom in Data Table B. Recall that multiple pairs of bonding electrons in double and triple bonds must "point" to the same atom.

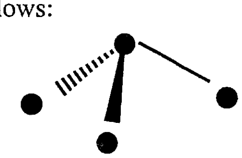
6. Use the following terms to describe the *molecular geometry* for each model: Linear, trigonal planar, bent, tetrahedral, pyramidal, trigonal bipyramidal, octahedral, square pyramidal, and square planar. Record the molecular geometry in Data Table B. *Hint:* Molecular geometry describes the physical arrangement of the atoms, not the electron pairs.

7. *Return to the molecules and polyatomic ions listed in Data Table A.* Refer to the models from Part B for comparison: Count the number of valence electron pairs (see step 4) around the central atom and predict the molecular geometry for each molecule or ion in Data Table A.

8. Draw a three-dimensional sketch of the molecule or ion in the space below its name and describe its molecular geometry (see step 6) in Data Table A. *Example:* The structure of H_2O could be sketched as follows:



The structure of H_3O^+ could be sketches as follows:



Name: ______________________________

Lewis Structures and Molecular Geometry

Data Table A

Name	Molecular Formula	Valence Electrons	Lewis Structure
Boron Trichloride			
Methane			
Ethylene	C_2H_4		
Ammonia			
Ammonium Ion			
Hydrogen Sulfide			

Name: ______________________________

Data Table A (continued)

Name	Molecular Formula	Valence Electrons	Lewis Structure
Sulfur Trioxide			
Acetylene	C_2H_2		
Phosphorus Trichloride			
Carbon Tetrachloride			
Iodine Pentafluoride			
Carbonate Ion			
Thiocyanate Ion	SCN^-		

Name: ______________________________

Data Table A (continued)

Name	Molecular Formula	Valence Electrons	Lewis Structure
Carbon Disulfide			
Formaldehyde	H_2CO		
Sulfate Ion			
Arsenic Pentafluoride			
Hydrogen Cyanide			
Sulfur Hexafluoride			
Xenon Tetrafluoride			

Name: ______________________________

Data Table B

Model	Bonding Pairs*†	Unshared Pairs*	Total Pairs	Sketch and Molecular Geometry
A				
B				
C				
D				
E				
F				
G				
H				
I				
J				
K				

*Count the bonding and nonbonding pairs of electrons around the central atom only.

†In the case of double or triple bonds, count all of the electrons involved in the bond as one pair of electrons.