

Name \_\_\_\_\_ Section \_\_\_\_\_

## EXPERIMENT 12: MOLECULAR ARCHITECTURE

### PRE-LABORATORY QUESTIONS

The following preparatory questions should be answered before coming to lab. They are intended to introduce you to several ideas important to aspects of the experiment. **You must turn in your work to your instructor before you will be allowed to begin the experiment.**

1. Give the total number of electrons and write the electron configurations for the following elements:
  - a. O
  
  
  
  
  
  
  
  
  
  
  - b. Al
  
  
  
  
  
  
  
  
  
  
  - c. Ca
  
  
  
  
  
  
  
  
  
  
  - d. Sn
  
  
  
  
  
  
  
  
  
  
  - e. Bi

2. Give the number of valence electrons and draw the Lewis structures for the following elements:

a. O

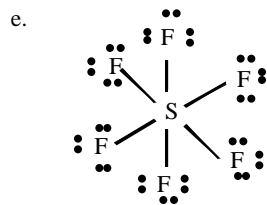
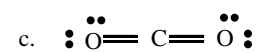
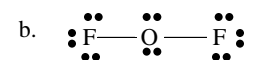
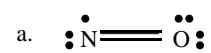
b. Al

c. Ca

d. Sn

e. Bi

3. Tell whether or not the following molecules satisfy the octet rule.



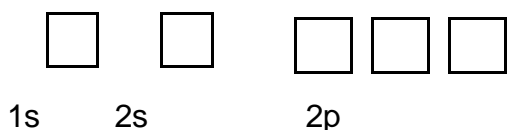
## EXPERIMENT 12: MOLECULAR ARCHITECTURE

### INTRODUCTION

The key to explaining the physical and chemical properties of a molecule lies in gaining an understanding of the bonding of its atoms and its structural shape. Today computers can perform very accurate and sophisticated calculations of molecular geometry that can be translated into visual images on a terminal using computer graphics. These images can be rotated so that we can view them from any angle. However, building molecules with molecular model kits can also help you to visualize the connections of atoms of molecules in three-dimensional space and it is these types of models that you will use during the lab.

#### Electronic Structure of Atoms

The electronic structure of an atom can be represented by either electron configuration notation or by an orbital diagram. For example, the electron configuration of a boron atom is  $1s^2 2s^2 2p^1$  and its orbital diagram is



#### Covalent Chemical Bonds

A covalent bond can be described as a pair of electrons shared by two atoms. The total number of outer orbital electrons of an atom, called its **valence electrons**, largely determines how many bonds that atom can form. For example, boron is in Group III A of the periodic table, has 3 valence electrons and can form 3 bonds.

#### Lewis Structures and the Octet Rule

A **Lewis structure** is simply a dot drawing that shows the arrangement of valence electrons around individual atoms and molecules. Each dot symbolizes a single valence electron and the appropriate number of dots is drawn around the chemical symbol(s) of the atom(s). Atoms in covalent bonds share electrons to achieve the same number of electrons as the noble gas that is closest to them in the periodic table. Because all noble gases (except He) have eight valence electrons, these atoms tend to share electrons until they are surrounded by eight valence electrons. This is known as the **octet rule**. Of course, because He has only two electrons, atoms near it in the periodic table, such as H, tend to obtain an arrangement of two electrons. There are many exceptions to the octet rule. A molecule can have less than an octet, an expanded octet, or contain an odd number of valence electrons. Some molecules cannot be represented with a single Lewis structure and must be represented by an average of two or more Lewis structures called **resonance** forms. All

resonance structures are equivalent and differ only in the arrangement of electrons, not the arrangement of the nuclei. The molecule's true structure is a blend of all the possible resonance structures.

### Rules for Drawing Lewis Structures

1. Sum the valence electrons from all atoms. For an anion, add an electron to the total for each negative charge. For a cation, subtract an electron for each positive charge.
2. Write the symbols for the atoms to show which atoms are attached to which, and connect them with a single bond. Atoms are often written in the order in which they are connected in the molecule or ion.
3. Complete the octets of the atoms bonded to the central atom.
4. Place any leftover electrons on the central atom, even if doing so results in more than an octet.
5. If there are not enough electrons to give the central atom an octet try multiple bonds. Use one or more of the unshared pairs of electrons on the atoms bonded to the central atom to form double or triple bonds.

### Valence Shell Electron Pair Repulsion Theory

Lewis structures are two-dimensional and cannot be used to predict a molecule's three-dimensional structure. VSEPR theory can. The basis of the VSEPR theory is that pairs of electrons in the valence shell of an atom will try to get as far away from each other as possible. Unshared electrons on a central atom are called **lone pairs** and shared electron pairs are called **bond pairs**. A double bond or a triple bond is counted as one bonding pair. A single electron is counted as a lone pair. The total number of electron pairs determines the **electron-pair geometry**, whereas only the atoms we see determine the **molecular shape**.

### Polarity

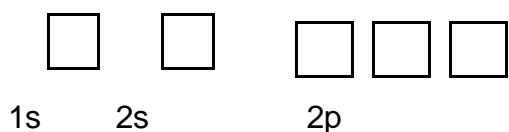
Once a molecule's three-dimensional structure is determined, its degree of polarity can be estimated. The concept of bond polarity is useful in describing the sharing of electrons between atoms. A **nonpolar** bond is one in which the electrons are shared equally between the 2 atoms. In a **polar** covalent bond, one of the atoms exerts a greater attraction for the electrons than the other. Degree of polarity is measured by the magnitude of the difference in **electronegativity** values between the bonded atoms. The greater an atom's electronegativity value, the greater is its ability to attract electrons to itself. Below are the electronegativity values for representative elements. In general, if the difference in the electronegativities of the 2 atoms in a bond is less than 0.5, the bond is considered nonpolar; if between 0.5 and 2.0, it is considered polar.

carbon	2.5
chlorine	3.0
oxygen	3.5
nitrogen	3.0
sulfur	2.5
hydrogen	2.1

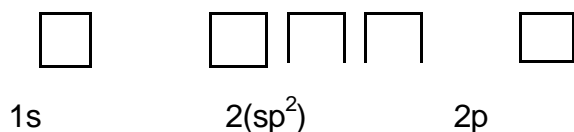
A symmetric molecule will be nonpolar even though it may contain polar bonds.

### Hybridization

Hybridization of orbitals is a concept required by valence bond theory to account for the fact that in some molecules more bonds are formed than would be expected from the predicted electron configuration of the atoms involved. This approach suggests that some of the atomic orbitals on the central atom are changed during the bonding process to give a new set of hybrid atomic orbitals, all exactly alike, suitable for bonding. For example, consider the  $\text{BH}_3$  molecule. The electron configuration of the central boron atom is  $1s^2 2s^2 2p^1$ , and the orbital diagram is



The p orbital contains only one unpaired electron; not enough to form 3 bonds. The orbital diagram of a hybridized B atom is as follows:



Three new  $sp^2$  orbitals are present and each has one electron. There are now enough unpaired electrons to form 3 covalent bonds. The 3 bonds are formed by overlap of the orbitals from 3 H atoms with the orbitals of the 3  $sp^2$  hybridized B atoms. Thus, B may form 3 bonds, although "normal" B has only one unpaired electron.

## EQUIPMENT NEEDED

### FROM THE STOREROOM

one molecular model kit (per pair of students)

## PROCEDURE

1. Each pair of students should obtain a molecular model kit from the storeroom.
2. Remove the pieces from the bag and make sure that the following tetrahedral centers are present

2 black	carbon
6 green	chlorine
4 blue	oxygen
2 red	nitrogen
1 yellow	sulfur

There should also be 8 white, single-bonded atoms representing hydrogen and 18 1-inch plastic connectors which represent a pair of electrons (either a lone pair or a bond pair).

3. Tear out the RESULTS pages before beginning.
4. For the first molecule, draw the Lewis structure, then build the model of the molecule using the kit. Your instructor will be circulating through the laboratory to see your Lewis structures and models-in-progress.
5. Once the model is built, look at it carefully and fill in the answers and other requested information about the molecule. This includes the total number of valence electrons, number of bond pairs, number of lone pairs, number of sigma bonds, number of pi bonds, the electron pair geometry, the molecular geometry and whether the molecule is polar or nonpolar.
6. Repeat the procedure for the remaining 11 molecules.

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**RESULTS** (The choices for electron pair geometry and molecular shape are linear, bent, trigonal planar, trigonal pyramidal, and tetrahedral)

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name: chlorine		bond pairs _____
Formula: Cl <sub>2</sub>		lone pairs _____
		sigma bonds _____
		pi bonds _____
		electron pair geometry _____
		molecular shape _____
		polar or nonpolar _____

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name: hydrochloric acid		bond pairs _____
Formula: HCl		lone pairs _____
		sigma bonds _____
		pi bonds _____
		electron pair geometry _____
		molecular shape _____
		polar or nonpolar _____

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name: carbon tetrachloride		bond pairs _____
Formula: CCl <sub>4</sub>		lone pairs _____
		sigma bonds _____
		pi bonds _____
		electron pair geometry _____
		molecular shape _____
		polar or nonpolar _____

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name: chloroform		bond pairs _____
Formula: CHCl <sub>3</sub>		lone pairs _____
		sigma bonds _____
		pi bonds _____
		electron pair geometry _____
		molecular shape _____
		polar or nonpolar _____

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name:		bond pairs _____

hydrogen cyanate  
Formula: HNCN

lone pairs \_\_\_\_\_  
sigma bonds \_\_\_\_\_  
pi bonds \_\_\_\_\_  
electron pair geometry \_\_\_\_\_  
molecular shape \_\_\_\_\_  
polar or nonpolar \_\_\_\_\_

Molecule or Ion  
Name:  
hydrogen sulfide  
Formula: H<sub>2</sub>S

Lewis Structure

valence electrons \_\_\_\_\_  
bond pairs \_\_\_\_\_  
lone pairs \_\_\_\_\_  
sigma bonds \_\_\_\_\_  
pi bonds \_\_\_\_\_  
electron pair geometry \_\_\_\_\_  
molecular shape \_\_\_\_\_  
polar or nonpolar \_\_\_\_\_

Molecule or Ion  
Name:  
formaldehyde  
Formula: H<sub>2</sub>CO

Lewis Structure

valence electrons \_\_\_\_\_  
bond pairs \_\_\_\_\_  
lone pairs \_\_\_\_\_  
sigma bonds \_\_\_\_\_  
pi bonds \_\_\_\_\_  
electron pair geometry \_\_\_\_\_  
molecular shape \_\_\_\_\_  
polar or nonpolar \_\_\_\_\_

Molecule or Ion  
Name:  
hydrazine  
Formula: N<sub>2</sub>H<sub>4</sub>

Lewis Structure

valence electrons \_\_\_\_\_  
bond pairs \_\_\_\_\_  
lone pairs \_\_\_\_\_  
sigma bonds \_\_\_\_\_  
pi bonds \_\_\_\_\_  
electron pair geometry \_\_\_\_\_  
molecular shape \_\_\_\_\_  
polar or nonpolar \_\_\_\_\_



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<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name:		bond pairs _____
sulfur dichloride		lone pairs _____
Formula: $\text{SCl}_2$		sigma bonds _____
		pi bonds _____
	electron pair geometry _____	
	molecular shape _____	
	polar or nonpolar _____	

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name:		bond pairs _____
carbonyl sulfide		lone pairs _____
Formula: $\text{COS}$		sigma bonds _____
		pi bonds _____
	electron pair geometry _____	
	molecular shape _____	
	polar or nonpolar _____	

<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name:		bond pairs _____
chlorite ion		lone pairs _____
Formula: $\text{ClO}_2^-$		sigma bonds _____
		pi bonds _____
	electron pair geometry _____	
	molecular shape _____	
	polar or nonpolar _____	

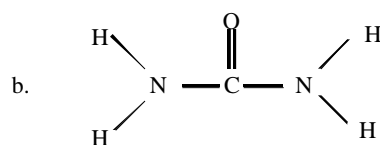
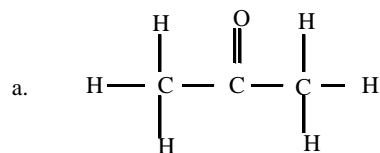
<u>Molecule or Ion</u>	<u>Lewis Structure</u>	valence electrons _____
Name:		bond pairs _____
hydronium ion		lone pairs _____
Formula: $\text{H}_3\text{O}^+$		sigma bonds _____
		pi bonds _____
	electron pair geometry _____	
	molecular shape _____	
	polar or nonpolar _____	

**Sign-out:**

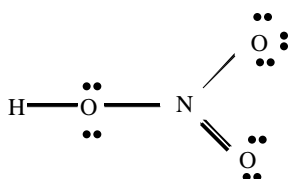
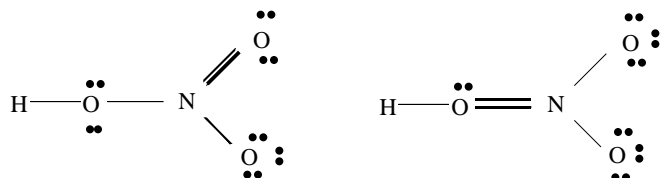
TA \_\_\_\_\_ Date \_\_\_\_\_

**POST LABORATORY QUESTIONS**

1. Finish drawing the Lewis structures of the following molecules and then tell how many sigma and pi bonds and how many bond pairs and lone pairs there are in each.

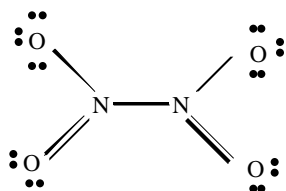


2. Which of the following is not a likely Lewis structure for  $\text{HNO}_3$ ? Why?



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3. A Lewis structure for  $\text{N}_2\text{O}_4$  is shown below. How many other resonance forms are possible? Draw them.



4. Predict the molecular geometry of each of the following molecules and state whether each is polar or nonpolar

a.  $\text{CO}_2$

b.  $\text{CH}_2\text{O}$

c.  $\text{HOCl}$

5. What hybridization is expected on the central atom of each of the following molecules?

a.  $\text{CH}_2\text{Br}_2$

b.  $\text{BeH}_2$

c.  $\text{BF}_3$