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

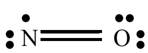
    b. Al

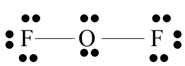
    c. Ca

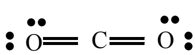
    d. Sn

    e. Bi

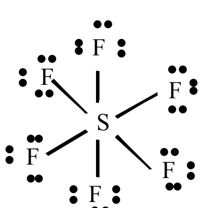
3. Tell whether or not the following molecules satisfy the octet rule.

    a. 

    b. 

    c. 

    d. 

    e. 

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

1s	2s	2p		
$\boxed{\uparrow\downarrow}$	$\boxed{\uparrow\downarrow}$	$\boxed{\uparrow}$	$\boxed{\uparrow}$	$\boxed{\uparrow}$

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 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.

<u>Hybridization</u>

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 BH_3 molecule. The electron configuration of the central boron atom is $1s^2\ 2s^2\ 2p^1$, and the orbital diagram is

$\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$

1s 2s 2p

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:

$\boxed{\uparrow\downarrow}$ $\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$ $\boxed{}$

1s $2(sp^2)$ 2p

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)

Molecule or Ion | Lewis Structure
Name:
chlorine
Formula: Cl_2

valence electrons ____________________
bond pairs ___________________________
lone pairs ___________________________
sigma bonds _________________________
pi bonds ____________________________
electron pair geometry ________________
molecular shape _____________________
polar or nonpolar ____________________

Molecule or Ion | Lewis Structure
Name:
hydrochloric acid
Formula: HCl

valence electrons ____________________
bond pairs ___________________________
lone pairs ___________________________
sigma bonds _________________________
pi bonds ____________________________
electron pair geometry ________________
molecular shape _____________________
polar or nonpolar ____________________

Molecule or Ion | Lewis Structure
Name:
carbon tetrachloride
Formula: CCl_4

valence electrons ____________________
bond pairs ___________________________
lone pairs ___________________________
sigma bonds _________________________
pi bonds ____________________________
electron pair geometry ________________
molecular shape _____________________
polar or nonpolar ____________________

Molecule or Ion | Lewis Structure
Name:
chloroform
Formula: $CHCl_4$

valence electrons ____________________
bond pairs ___________________________
lone pairs ___________________________
sigma bonds _________________________
pi bonds ____________________________
electron pair geometry ________________
molecular shape _____________________
polar or nonpolar ____________________

Molecule or Ion | Lewis Structure
Name:

valence electrons ____________________
bond pairs ___________________________

hydrogen cyanate
Formula: HNCO

lone pairs ______________________________
sigma bonds ______________________________
pi bonds ______________________________
electron pair geometry __________________
molecular shape ________________________
polar or nonpolar ________________________

Molecule or Ion
Name:
hydrogen sulfide
Formula: H_2S

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_2CO

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_2H_4

Lewis Structure

valence electrons ______________________
bond pairs ______________________________
lone pairs ______________________________
sigma bonds ______________________________
pi bonds ______________________________
electron pair geometry __________________
molecular shape ________________________
polar or nonpolar ________________________

Name ______________________________ Section ______________________________

Molecule or Ion | Lewis Structure | valence electrons ______________________
Name:
sulfur dichloride
Formula: SCl_2

bond pairs ______________________________
lone pairs ______________________________
sigma bonds ___________________________
pi bonds ______________________________
electron pair geometry _________________
molecular shape _______________________
polar or nonpolar ______________________

Molecule or Ion | Lewis Structure | valence electrons ______________________
Name:
carbonyl sulfide
Formula: COS

bond pairs ______________________________
lone pairs ______________________________
sigma bonds ___________________________
pi bonds ______________________________
electron pair geometry _________________
molecular shape _______________________
polar or nonpolar ______________________

Molecule or Ion | Lewis Structure | valence electrons ______________________
Name:
chlorite ion
Formula: ClO_2^-

bond pairs ______________________________
lone pairs ______________________________
sigma bonds ___________________________
pi bonds ______________________________
electron pair geometry _________________
molecular shape _______________________
polar or nonpolar ______________________

Molecule or Ion | Lewis Structure | valence electrons ______________________
Name:
hydronium ion
Formula: H_3O^+

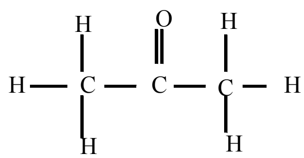
bond pairs ______________________________
lone pairs ______________________________
sigma bonds ___________________________
pi bonds ______________________________
electron pair geometry _________________
molecular shape _______________________
polar or nonpolar ______________________

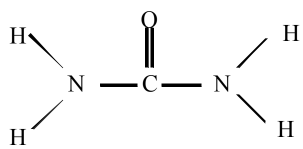
Sign-out:

TA ________________________________ Date ______________________

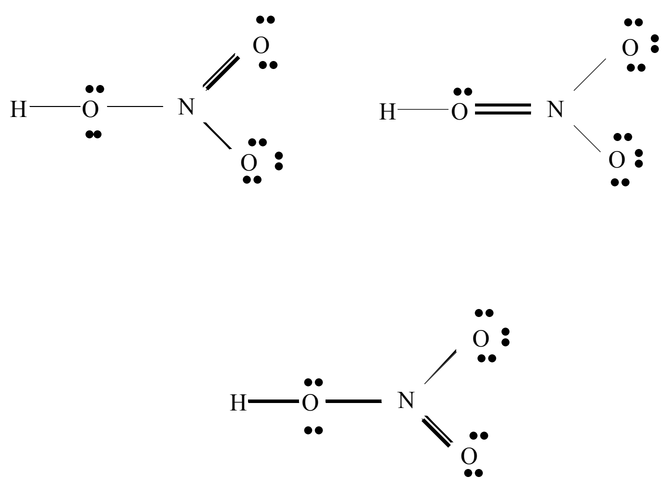
POST LABORATORY QUESTIONS

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.

a. 

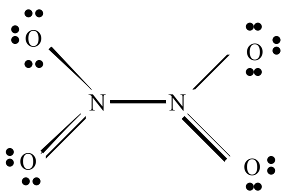
b. 

2. Which of the following is <u>not</u> a likely Lewis structure for HNO_3 ? Why?



Name ______________________________ Section ______________________

3. A Lewis structure for N_2O_4 is shown below. How many other resonance forms are possible? Draw them.



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

a. CO_2

b. CH_2O

c. HOCl

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

a. CH_2Br_2

b. BeH_2

c. BF_3