

Fill-in, stamp the box on top of page 7.

Name _____

Partner _____

Lecture Instructor _____

Date _____

Turn in ONLY pages 7–10!!!!**LEARNING OBJECTIVES** *After completing this exercise, you should feel comfortable with:*

- Drawing Lewis structures for molecules that obey the octet rule.
- Drawing Lewis structures for molecules that may violate the octet rule.
- Visualizing the three-dimensional shape of a molecule based on a drawing.
- Identifying electron pair geometries (VSEPR).
- Applying VSEPR theory to determine the shapes of molecules.
- Identifying molecular geometries.
- Distinguishing between electronic and molecular geometries.
- Applying valence bond theory to the hybridization of atomic orbitals.

TO EARN YOUR FINAL STAMP: *The following items must be completed to earn the final stamp. You may complete the entire assignment in lab or outside of the lab, this reflect the minimum required to earn your final stamp.*

- Complete the entire worksheet. You may work on the worksheet outside of the lab, however you **MUST** have it completed all tables to get a stamp. The lab instructor will check over your worksheet when you get it stamped.

Introduction

Because atoms are too small to see with the eye, scientists use models to visualize the physical arrangements of atoms in molecules and polyatomic ions. These three-dimensional models aid in understanding the polarity, reactivity and interaction of molecules. In this laboratory exercise, you will work with three related theories of molecular bonding and structure.

I. LEWIS STRUCTURES

Lewis Structures give information in two-dimensional representations that can be used to predict the three dimensional shapes of molecules and ions.

A basic concept of the atomic theory is that the chemical and physical properties of a substance are determined by the distribution of outer shell or valence electrons (highest "n" value) in its atoms and by the arrangements of these atoms to each other. The extraordinary non-reactivity of the Noble gases has been related to their common electronic configuration of eight valence electrons (an "octet"). Many chemical reactions and molecular formulas can be related to the observation that many elements would "like" to have the same electronic configuration as the Noble gases.

The following rules and procedures are given as a guide for drawing Lewis Dot Structures.

1. Write the **MOLECULAR FORMULA** for the compound.
2. Determine the total number of **VALENCE ELECTRONS** available for bonding by:
 - a. counting the valence electrons from each element in the compound.
 - b. adding one electron for each **negative** charge or subtracting one electron for each **positive** charge, for polyatomic ions
3. **ARRANGE ATOMS.** For small molecules and polyatomic ions, place the element with the lowest electronegativity in the center and arrange the other atoms around this central atom using the following rules:
 - a. Hydrogen is never the central atom.
 - b. For oxyacids, the hydrogen atoms are usually bonded to oxygen atoms that are bonded to the less electronegative central atom.
4. **CONNECT ATOMS.** Attach the atoms together with a "—" to signify a two-electron bond between the atoms.
5. **SATISFY OCTET RULE.** Place the remaining electrons, in pairs (lone pairs), around each atom to satisfy the "octet" requirement (a "duet" for hydrogen). It is best to maximize bonding; if all of the electrons have been used up without satisfying the octet rule then atoms must share more electrons by forming another bond. The octet rule **must apply for C, N, O and F!** For all others, it is a good guideline, but may be violated (see item #6)
6. **EXCEPTIONS TO OCTET RULE:** There are some compounds that contain elements with exceptions to the octet rule. These may have more than eight electrons, typically when $n \geq 3$ (PCl_5), or less than eight electrons, typically Group IIA, (BeCl_2), IIIA (BCl_3), and, of course, hydrogen. For most of the compounds, the atoms are bonded by single bonds consisting of one electron from the central atom and one electron from the outer atom. If there are any extra electrons, they are placed on the central atom as unshared, or lone, pairs.

II. VALENCE SHELL ELECTRON PAIR REPULSION (VSEPR)

VSEPR theory states that regions of high electron density, such as bonding pairs or lone pairs of electrons (a VSEPR or electron domain), will arrange themselves as far apart as possible around the central atom. Each single, double, or triple bond or unshared pair is counted as an electron domain.

The VSEPR rules:

1. Write the **LEWIS STRUCTURE**.
2. Count the number of **ELECTRON DOMAINS** around the central atom (or any atom!).

(Single, double, triple bonds = 1 VSEPR domain)

(Non-bonding (lone) pairs of electrons = 1 VSEPR domain)
3. Pick the **VSEPR/ELECTRONIC GEOMETRY**. Note that this electronic geometry is based only on the number of electron domains, regardless of what they are (triple bond, lone pair, etc...). Consult Table 1 to assign these geometries and the corresponding bond angles.

(Arrange the VSEPR pairs to minimize repulsion)

Table 1: VSEPR Electronic Geometries

Number of Electron Domains	VSEPR/Electronic Geometry	Ideal Bond Angle(s)
2	Linear	180°
3	Trigonal Planar	120°
4	Tetrahedral	109.5°
5	Trigonal Bipyramidal	180°/120°/90°
6	Octahedral	180°/90°

4. Determine the **MOLECULAR GEOMETRY**. The molecular geometry is determined by what we can actually “see” – the atoms bonded to the central atoms, but not the lone pairs. The molecular geometry is set by the electronic geometry. Consult Table 2 to assign these geometries

(Account for any unfilled positions in the electron pair geometry, i.e. non-bonding pairs/lone pairs)

Table 2: VSEPR Molecular Geometries

Total # of e ⁻ domains	Number of non-bonding or lone pairs on an atom			
	0	1	2	3
2	Linear			
3	Trigonal Planar	Bent	Linear	
4	Tetrahedral	Trigonal Pyramidal	Bent	
5	Trigonal Bipyramidal	See-Saw	T-Shaped	Linear
6	Octahedral	Square Pyramidal	Square Planar	T-shaped

5. Adjust angles to Recognize **STERIC (size) EFFECTS**. This gives rise to slight deviations to the ideal bond angles.

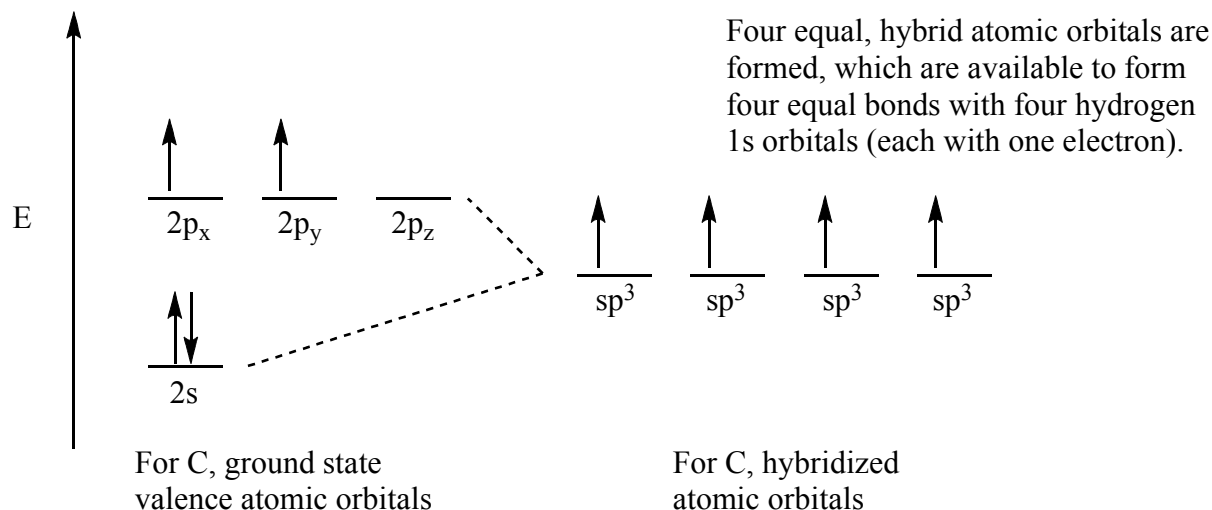
Multiple Bonds – double, triple bonds take up more space than single bonds, therefore angles involving them will be somewhat larger.

Non-Bonding/Lone Pairs – Lone Pair electrons take up much more space than bonding pairs, compressing the angles between other, bonding pairs.

The molecular geometries (the actual geometry of the atoms) might best be explained with the diagrams in your text.

III. VALENCE BOND THEORY

Valence bond theory attempts to explain the number of bonds carbon forms and the shapes of molecules by mixing, or hybridizing, the atomic orbitals on the central atom before the orbitals overlap with other atoms and form bonds and molecular orbitals. This is explained by combining pure atomic orbitals of different energies and redistributing them into hybrid atomic orbitals of equal energy. These new hybrid orbitals are of intermediate energy – they fall in between the energies of the original orbitals. The electrons are then returned to the new hybrid orbitals according to Hund's Rule. Once the hybrid orbitals are formed, they can now accept electrons from other atoms in order to form bonds. Let's look at the valence orbitals for carbon in CH₄.



The number of hybrid atomic orbitals *must* equal the number of atomic orbitals used to make the hybrid orbitals: One 2s and three 2p orbitals form four sp³ hybrid orbitals.

Four atomic orbitals become four hybrid molecular orbitals. These hybrid orbitals then interact with the electrons in the Hydrogen 1s orbitals for make 4 equivalent bonds.

Consult Table 3 to determine the hybridization of the central atom, based on VSEPR electronic domains.

Table 3: Hybridization

# of VSEPR domains	2	3	4	5	6
Electronic Geometry	linear	trigonal planar	tetrahedral	trigonal bipyramidal	octahedral
Hybridization	sp	sp ²	sp ³	sp ³ d	sp ³ d ²
Ideal Bond Angles	180°	120°	109.5°	90°, 120°, 180°	90°, 180°

The following example shows the complete process of drawing a Lewis structure for a molecule and determining the electronic geometry, molecular geometry, hybridization of the central atom and the ideal bond angle(s).

Example 1: From the molecular formula for nitrite, NO_2^{-1} determine the Lewis structure, VSEPR (electronic) geometry, hybridization, molecular shape and ideal bond angles

Drawing the Lewis Structure

Step 1: Determine the number of valence electrons total in the structure

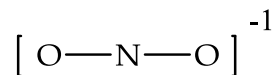
$$\text{N: } 1 \times 5 = 5 \text{ and O: } 2 \times 6 = 12$$

Total = 17 but it is a negatively charged ion so we must add 1 more electron for a **total of 18 valence electrons**.

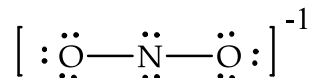
Step 2: Put the least electronegative atom in the center, and “err” on the side of symmetry (meaning, nature likes symmetry so make the atoms in the structure symmetrical). Connect the central atom to the others with a ‘-’ indicating a bond for two electrons.



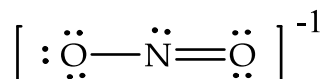
This is an ion – an easy way to indicate this is to place the structure in brackets and put the charge on the outside of the bracket



Step 3: Give all atoms an octet by placing lone pair electrons around all species



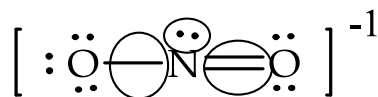
Step 4: Count up the electrons on your structure – if you have the same number of electrons as previously counted in step 1, you have a valid Lewis structure that follows the octet rule. In this example, if we count up the number of electrons, we see that we have put 20 electrons (!!) on the structure. Too many electrons on a structure means that you most likely need to include double or triple bonds. To reduce the number of electrons in the structure *and* maintain octets around the atoms you can add a second bond between two atoms and remove a lone pair of electrons from *each* atom on the double bond. You cannot simply erase electrons – because then your species do not have an octet!



Step 5: Do another count of electrons, optimizing bonding and maintaining octets until the correct number of valence electrons is represented in the structure. This structure now has 18 e^- – which is what we need! In addition, each atom still ‘feels’ as if it has 8 e^- surrounding it.

Determining the VSEPR/Electronic Geometry and Ideal Bond Angle

Count up the electron domains around the central atom (N) – all single, double, triple bond, and lone pairs all count as ONE domain.



On this structure, there are 3 electron domains around the N. Using the Table 1 (partially copied here for convenience), we see that if there are 3 electron domains, the VSEPR shape will be **trigonal planar**, with a **120°** bond angle

Number of Electron Domains	VSEPR/Electronic Geometry	Ideal Bond Angle(s)
2	Linear	180°
3	Trigonal Planar	120°
4	Tetrahedral	109.5°

Determining the Molecular Shape/Geometry

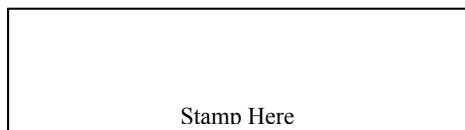
This shape is based on the electron domains/VSEPR shape. We see that our structure has two bonding domains (where there are bonds!) and one lone-pair (or non-bonding) domain. Therefore, examining Table 2 (partially copied here for convenience), we use the VSEPR shape with three total domains (3rd row) and with 1 non-bonding domain (3rd column) and see a molecular shape of **bent**.

Total # of e ⁻ domains	Number of non-bonding or lone pairs on an atom			
	0	1	2	3
2	Linear			
3	Trigonal Planar	Bent	Linear	
4	Tetrahedral	Trigonal Pyramidal	Bent	

Determining the Hybridization

Again, this is based off the number of electron domains. Using table 3, we have three total electron domains (3rd column) so we see we have **sp² hybridization**

# of VSEPR domains	2	3	4	5	6
Electronic Geometry	linear	trigonal planar	tetrahedral	trigonal bipyramidal	octahedral
Hybridization	sp	sp ²	sp ³	sp ³ d	sp ³ d ²



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Procedure: In this experiment you will draw Lewis structures for a series of molecules and determine the electronic (VSEPR) geometry, hybridization, molecular geometry and ideal bond angle(s) **for the central atom or other specified atom**. *Molecules marked with an asterisk do not obey the octet rule. You may use marshmallows and toothpicks, or molecular models (available in the lab) to help visualize the actual geometry. The octet rule **must apply for C, N, O and F!** For all others, it is a good guideline, but may be violated.

Molecular Formula	Lewis Structure	Electronic Geometry	Hybridization	Molecular Geometry	Ideal Bond Angles
NH_3 $5+3(1)=8e^-$ (# valence e^-)	$\begin{array}{c} \text{H} - \overset{\cdot\cdot}{\text{N}} - \text{H} \\ \\ \text{H} \end{array}$	tetrahedral	sp^3	trigonal pyramid	109.5°
H_2O					
CH_2Cl_2					
$*\text{OPCl}_3$ (violate octet rule)					

Molecular Formula	Lewis Structure	Electronic Geometry	Hybridization	Molecular Geometry	Ideal Bond Angles
CO_3^{2-}					
* AlCl_6^{3-} (violate octet rule)					
* SO_2 (violate octet rule)					
* SO_4^{2-} (violate octet rule)					

Molecular Formula	Lewis Structure	Electronic Geometry	Hybridization	Molecular Geometry	Ideal Bond Angles
<p style="text-align: center;">*ICl₄⁻ (violate octet rule)</p>					
<p style="text-align: center;">*BrF₃ (violate octet rule)</p>					
<p style="text-align: center;">*SeF₄ (violate octet rule)</p>					
<p style="text-align: center;">*BrF₅ (violate octet rule)</p>					

Molecular Formula	Lewis Structure	Electronic Geometry	Hybridization	Molecular Geometry	Ideal Bond Angles
*PCl ₅ (violate octet rule)					
CH ₂ O		C	C	C	C
C ₂ H ₆ O (CH ₃ OCH ₃)		C O C	C O C	C O C	C O C
C ₂ H ₆ O (C ₂ H ₅ OH)		C C O	C C O	C C O	C C O
C ₆ H ₆ (C's form a ring)		One C only			