

Week 4 Assignment a, b, and c

Atomic Structure, Chemical Bonding, Lewis Structure, and 3D Molecular Shape

Objectives

In this lab, you will apply valence bond theory to draw appropriate Lewis structures, use electronegativity differences to classify bonds as ionic, polar covalent, or nonpolar covalent, and apply valence shell electron pair repulsion theory (VSEPR) to predict molecular geometry. We will also use molecular kits to create ball and stick models of molecules of interest to you.

Theory

Atoms of certain species tend to bond together. An atom is more stable if its valence shell (electrons in its outermost energy level) is similar to that of a Noble Gas (typically eight electrons), and this number is most often achieved when atoms combine. Notice that atoms of elements in the same group on the periodic table tend to have the same number of valence electrons; for example, halogens, Group 7A elements (**Figure 1**), have seven valence electrons.

	Group 1A	Group 2A	Group 3A	Group 4A	Group 5A	Group 6A	Group 7A	Group 8A
Period 1	•H							:He
Period 2	•Li	•Be	•B•	•C•	:N•	:O•	:F:	:Ne:
Period 3	•Na	•Mg	•Al•	•Si•	:P•	:S•	:Cl:	:Ar:
Period 4	•K	•Ca	•Ga•	•Ge•	:As•	:Se•	:Br:	:Kr:
Period 5	•Rb	•Sr	•In•	•Sn•	:Sb•	:Te•	:I:	:Xe:
Period 6	•Cs	•Ba	•Tl•	•Pb•	:Bi•	:Po•	:At:	:Rn:
Period 7	•Fr	•Ra						

Figure 1: Dot Diagrams

For most elements, a full outer energy level has eight electrons, *an octet*. The elements in group 8A have a full outer energy level. Helium (He), in period 1, is an exception, requiring only two electrons. Because group 8A elements' atoms already have a full outer energy level, those elements tend to be nonreactive—they rarely combine with other atoms to form compounds. Atoms can fill their outer energy level by transferring or sharing electrons to form either *ionic* or *covalent* compounds.

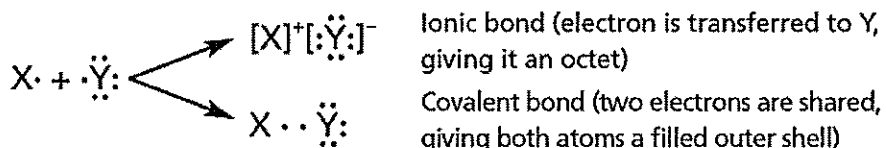


Figure 2: Two Bonding Types

Whether two given atoms tend to bond ionically or covalently is determined by the difference in their electronegativity. Electronegativity is a dimensionless number that is a measure of an atom's attraction for bonding valence electrons. Electronegativities show periodic trends on a periodic table.

Increasing electronegativity →									
1A	2A		3A	4A	5A	6A	7A	8A	
H 2.1									↑ Increasing electronegativity
Li 1.0	Be 1.5		B 2.0	C 2.5	N 3.0	O 3.5	F 4.0		
Na 0.9	Mg 1.2		Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0		
K 0.8	Ca 1.0		Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8		
Rb 0.8	Sr 1.0		In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5		

Figure 3: Table of Electronegativities

Excluding the noble gases, the most electronegative element is fluorine, which is assigned a value of 4.0. The other elements' values are calculated on the basis of that of fluorine. Across each period, electronegativities tend to increase. The nonmetal families of nitrogen, oxygen, and fluorine have the highest values. Due to their atoms' small radii, the positive nuclei exert a greater attraction for bonding electrons. The alkali metals and alkaline earth metals (the groups on the left side of the periodic table) have the lowest electronegativities because their atoms have the largest radii. Cesium (and francium – not shown in **Figure 3**), with the largest radii, have the lowest electronegativity, at 0.7.

Lewis Dot Structures

A Lewis dot structure is one way to represent the arrangement of valence electrons in a molecule (**Figure 1**). In Lewis structures, an element symbol is surrounded by a specific number of dots representing valence electrons. Most atoms obey the octet rule; they need eight valence electrons to fill their outer shell. (Exceptions include hydrogen and helium, which need only two. Also, boron and beryllium may form compounds with fewer than eight, and elements in periods 3–6 may use more than eight.)

To fill their outer shells, elements can form covalent bonds by sharing electrons. To show those bonds, Lewis structures are often used. Covalent compounds may have single, double, or triple bonds between atoms. These bonds are represented in a **Lewis structure** with dashes between the chemical symbols of the bonded elements. The number of dashes corresponds to the number of bonds. Lewis structures also indicate the **lone pairs** of electrons on different atoms. Use the guide below if it helps in drawing Lewis Structures.

Guidelines for Drawing Lewis Structures	Example SiO ₂
1. Determine the number of valence electrons present for each atom in the compound (consult Figure 1 in the background section as needed).	Silicon (Si): 4 valence electrons Oxygen (O): 6 valence electrons Oxygen (O): 6 valence electrons
2. Find the sum of valence electrons of all the atoms. If there is a charge on a compound, add an electron for each negative charge and subtract an electron for each positive charge.	Silicon (Si): 4 valence electrons Oxygen (O): 6 valence electrons Oxygen (O): + 6 valence electrons <u>16 total electrons</u>
3. Determine which atom is to be the central atom. This is typically the least electronegative element (that is not hydrogen) or the first element in the chemical formula. Note: Some compounds have no central atom; the first element in the formula is a good place to start.	Central atom: silicon
4. Write the chemical symbol of the central atom, followed by the chemical symbols for other atoms around it.	O Si O
5. Use dots to show the appropriate number of valence electrons around each symbol in the compound.	:Ö · ·Si· ·Ö:
6. Determine the total number of electrons required for each element. Allow for exceptions to the octet rule as needed.	Silicon (Si) needs 8 valence electrons. Oxygen (O) needs 8 valence electrons. Oxygen (O) needs 8 valence electrons.
7. Create a skeleton structure by connecting unpaired electrons from the central atom to unpaired electrons on the atoms around it with a solid line. Each solid line now represents a (two-electron) covalent bond between the two atoms.	:Ö=Si=Ö:
8. Redraw the structure as needed. If multiple bonds exist between two atoms, reorient the chemical symbols as needed.	Ö=Si=Ö or :Ö-Si≡Ö:
9. Sometimes there will be more than one way to add the bonds. To determine which Lewis structure is the best model, formal charge is often used. To determine the formal charge of atoms: a. Count the number of valence electrons that each atom typically has when unbonded. b. In the Lewis structure being evaluated, count the number of assigned electrons for an atom by counting the number of electrons that exist around that atom as lone pairs and then counting the number of covalent bonds on that atom. Add the number of lone pair electrons and the number of bonds together. c. Subtract the number of assigned electrons from the number of valence electrons. That value is the formal charge for the atom in that Lewis structure.	$\begin{array}{rcccc} & \text{Ö} & = & \text{Si} & = & \text{Ö} \\ \text{unbound electrons} & 6 & & 4 & & 6 \\ \text{assigned electrons} & -6 & & -4 & & -6 \\ \hline \text{formal charge} & 0 & & 0 & & 0 \end{array}$ $\text{:}\ddot{\text{O}}-\text{Si}\equiv\ddot{\text{O}}\text{:}$ $\begin{array}{rcccc} & 6 & 4 & 6 \\ \text{unbound electrons} & 6 & & 4 & & 6 \\ \text{assigned electrons} & -7 & & -4 & & -5 \\ \hline \text{formal charge} & -1 & & 0 & & +1 \end{array}$
10. Lewis structures should show negative charge on the most electronegative elements and positive charge on the least electronegative elements.	$\ddot{\text{O}}=\text{Si}=\ddot{\text{O}}$ the preferred structure of SiO ₂

Part a: Lewis Structures

Procedure

1. Select **two** compounds in Group 1, **two** compounds in Group 2, and **two** compounds in Group 3 to use in experiments 1, 2, and 3. You will focus on **these six compounds** in all three "experiments" (or activities) in today's lab.

Group 1	Group 2	Group 3
1. CH ₄	1. CO ₂	1. BH ₃
2. PCl ₃	2. NH ₃	2. BeCl ₂
3. PCl ₅	3. H ₂ O	3. CH ₃ OH
4. SF ₆	4. SF ₄	4. H ₂ CO

2. Copy each chemical formula chosen into the spaces provided in the first column of **Data Table 1**.
3. Use the Guidelines for Drawing Lewis Structures (*page 3*) to complete the Data Table 1.
4. For each group (**6 compounds in total**), ensure that you:
 - a. copied the chemical formula correctly.
 - b. drew dot diagrams that match those provided in Figure 1.
 - c. accounted for the correct number of each type of atom.
 - d. accounted for the correct number of electrons for each type of atom.
 - e. selected the appropriate central atom.
 - f. drew a Lewis structure that includes the appropriate number of electrons.

Name(s): _____

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Data Table 1 (Group 1):

Chemical Formula:	Central Atom:
Dot Diagrams of each element:	Total # of Electrons:
Lewis Structure (Dot structure) of the Molecule:	

Chemical Formula:	Central Atom:
Dot Diagrams of each element:	Total # of Electrons:
Lewis Structure (Dot structure) of the Molecule:	

Name(s): _____

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Data Table 1 (Group 2):

Chemical Formula:	Central Atom:
Dot Diagrams of each element:	Total # of Electrons:
Lewis Structure (Dot structure) of the Molecule:	

Chemical Formula:	Central Atom:
Dot Diagrams of each element:	Total # of Electrons:
Lewis Structure (Dot structure) of the Molecule:	

Data Table 1 (Group 3):

Chemical Formula:	Central Atom:
Dot Diagrams of each element:	Total # of Electrons:
Lewis Structure (Dot structure) of the Molecule:	

Chemical Formula:	Central Atom:
Dot Diagrams of each element:	Total # of Electrons:
Lewis Structure (Dot structure) of the Molecule:	

Part b: Molecular Geometry

In this experiment you will apply valence shell electron pair repulsion theory (VSEPR) to predict molecular geometry. Afterwards, you will construct three-dimensional molecular models, using small, pronged atoms and flexible bonds (included in the kits). Lastly, you will sketch a three-dimensional model of chemical structure using dashed lines and wedges for all of the 6 molecular compounds.

Procedure

1. For each of the **6 compounds in Data Table 1 (part a)**, determine how many electron domains are present on the central atom (use the Lewis structures of the 6 compounds from Experiment 1). Record the number of **electron domains** in the appropriate column in *Data Table 2* (below).
2. Next, again using your previous Lewis Structure, determine how many electron domains on the central atoms are **lone pairs**. Record your answer in the appropriate column of *Data Table 2* (below).
3. Once you have determined the number of electron domains and number of lone pairs, use the reference table below (**Figure 4**) to determine the appropriate molecular geometry (name and bond angles). Record your answer in *Data Table 2* (below).

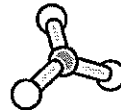
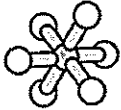
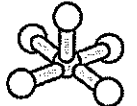
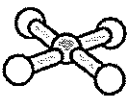
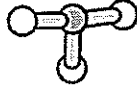
Electron Domains	No Lone Pairs	One Lone Pair	Two Lone Pairs	Three Lone Pairs
2 Geometry: Bond Angles:	 linear 180°			
3 Geometry: Bond Angles:	 trigonal planar 120°	 bent <120°		
4 Geometry: Bond Angles:	 tetrahedral 109.5°	 trigonal pyramidal 109.5°	 bent/angular 109.5°	
5 Geometry: Bond Angles:	 trigonal bipyramidal 90°, 120°	 see-saw 90°, 120°	 T-shaped 90°	 linear 180°
6 Geometry: Bond Angles:	 octahedral 90°	 square pyramidal 90°	 square planar 90°	 T-shaped 90°

Figure 4: Molecular Geometries

Name(s): _____

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Data Table 2:

Chemical Formula	# of Electron Domains around Central Atom	Number of lone pairs on the Central Atom	Molecular geometry and Bond Angles Example: Tetrahedral, 109.5 deg

Part c: Bonding and Polarity

In this experiment you will calculate electronegativity differences to determine bond type. Then, you will calculate molecular polarity and identify dipole moment.

Background

Although chemical bonds are characterized as covalent or ionic, they are rarely fully one type or the other. Few molecules are fully covalent, sharing valence electrons equally, and few are fully ionic, with a complete transfer of valence electrons. Instead, bonds are typically described on the basis of the character exhibited most; for example, the bond between a metal and a nonmetal has more ionic character than covalent and so is referred to as an ionic bond. The bond between two nonmetals is typically considered covalent. In a nonpolar covalent bond, electrons are shared equally. In a covalent bond with a certain amount of ionic character, the electrons are not really equally shared. The atom with the greater electronegativity attracts the electrons more strongly. This unequal sharing creates poles of charge, and thus these bonds are termed **polar** covalent bonds.

Because bonds usually fall somewhere between truly covalent and truly ionic, chemists sometimes use the terms percent ionic and percent covalent to describe the bonding between atoms. One way to calculate these percentages is to first determine the difference between the electronegativities of two atoms. If the electronegativity difference is greater than 1.9, the bond is considered more ionic than covalent and is characterized as ionic. If the difference is 1.9 or less, the bond is said to be covalent. An electronegativity difference between 1.9 and 0.5 indicates a **polar** covalent bond, while any bond polarity lower than 0.5 indicates a **nonpolar** covalent bond.

Electronegativity Difference	Bond Type	Electron Sharing
Less than 0.5 unit	Nonpolar	Electrons are equally shared.
0.5–1.9 units	Polar covalent	Electrons are unequally shared; they are pulled toward the more electronegative element.
Greater than 1.9 units	Ionic	Electrons are transferred from the less electronegative element to the more electronegative element.

Figure 5: Approximate ranges of bond polarity for Ionic, Polar Covalent, and Nonpolar Covalent bonds

Sample Bond Type Calculations

Bonding Pair	Electronegativity Difference	Type of Bond
Li and F	$ 1.0 - 4.0 = 3.0$	ionic
F and F	$ 4.0 - 4.0 = 0.0$	nonpolar covalent
C and F	$ 2.5 - 4.0 = 1.5$	polar covalent

Bond Polarity

The terms nonpolar and polar are useful descriptors for covalent bonds. A nonpolar covalent bond has no region (pole) of positive or negative charge. An example of this type of bond is the bond

between two identical atoms, as in H_2 . Because each hydrogen atom has one available electron, the electronegativity difference ($|2.1 - 2.1|$) equals 0. The two atoms exert the same amount of attraction on the electrons ($\text{H}\cdot\text{H}$).

In a polar covalent bond, one atom attracts the bonding electrons more strongly than the other does. The tendency of the electrons to be closer to one atom than the other creates the poles of charge. The atom with the stronger attraction has a partial negative charge, and the other has a partial positive charge. Consider hydrochloric acid, HCl . The electronegativity difference between chlorine and hydrogen is 0.9 ($|3.0 - 2.1| = 0.9$). Chlorine is more electronegative and therefore pulls the bonding electron pair more closely, giving the hydrogen a partial positive charge (delta plus, δ^+) and the chlorine a partial negative charge (delta minus, δ^-).

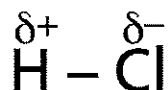


Figure 6: Hydrochloric acid, HCl , showing partial charges

Unequal sharing of electrons can be represented by a vector indicating bond polarity. To show bond polarity, draw a vector from the positively charged atom to the negatively charged atom. Create a plus sign using a vertical line near the less electronegative atom. The vector arrow points toward the more electronegative atom.



Figure 7: Hydrochloric acid, HCl , showing bond polarity

Molecular Polarity

Molecular polarity is similar to bond polarity. A polar molecule has regions of partial positive and negative charge, oriented in an electric field. The orientation, called a dipole moment, is caused by asymmetric distribution of charges within the molecule. The molecular dipole moment is shown as a vector beside the molecule. Once again, the vector arrow points toward the more electronegative atom.

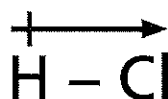


Figure 8: Hydrochloric acid, HCl , showing molecular dipole moment

Molecules that demonstrate a dipole moment are characterized as polar. Molecules of hydrochloric acid are polar because the bond polarity is unbalanced.

Not all molecules that contain polar covalent bonds are themselves polar. If bond polarity is balanced, partial positive and negative charges are distributed symmetrically. If positive and negative charges are distributed symmetrically, the molecule does not orient itself in an electric field and does not demonstrate a dipole moment. Molecules that do not demonstrate a dipole moment are characterized as nonpolar.

Beryllium chloride is an example of a nonpolar molecule that contains polar covalent bonds. Each Be–Cl bond is polar covalent with an electronegativity difference of 1.5 ($|1.5 - 3.0| = 1.5$). However, molecular geometry of beryllium chloride (linear) results in symmetrical bonds and a nonpolar molecule. Beryllium chloride does not have a dipole moment because the opposing bond polarities cancel each other.



Figure 9: Beryllium chloride, BeCl, showing bond polarity

It is also possible to arrange polar covalent bonds symmetrically in three-dimensional space. For example, in carbon tetrachloride, each C–Cl bond is a polar covalent one. The electronegativity difference is 0.5 ($|2.5 - 3.0| = 0.5$). The molecular geometry of carbon tetrachloride (tetrahedral) results in three-dimensional symmetry and a nonpolar molecule. Carbon tetrachloride does not have a dipole moment because the opposing bond polarities cancel each other.

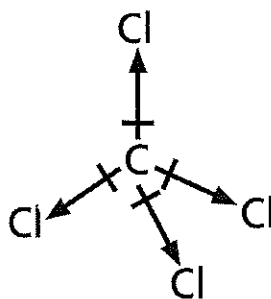


Figure 10: Carbon tetrachloride, CCl₄, showing cancelation of polar bonds

Polar molecules are the result of unbalanced bond polarity; consequently, all polar molecules are asymmetrical in some way. If one chlorine atom in carbon tetrachloride (CCl₄) is replaced with a hydrogen atom, the molecule becomes chloroform (CHCl₃). The tetrahedral molecule is no longer symmetric; it is asymmetric and polar. This molecule has a region of partial positive charge near the hydrogen atom and a region of negative charge near the chlorine atoms. The configuration results in a molecular dipole moment shown by the large vector on the far right.

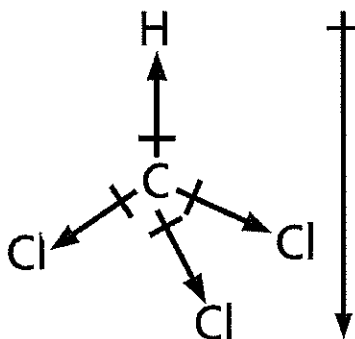


Figure 11: Chloroform, CHCl₃, a polar molecule

The presence of lone pairs of electrons contributes to the polarity of a molecule. Lone pairs are regions of partial negative charge; however, not all molecules that contain lone pairs are polar. The combination of molecular geometry and multiple lone pairs may result in a symmetric, nonpolar molecule.

Procedure

1. **Use the same 6 compounds from part a and b (Data Table 1 and 2).** Complete Data Table 3 (below), using the Periodic Table of the Electronegativities (**Figure 3**) and the Bonding Scale (**Figure 5**) to determine the type of bond each set of atoms would exhibit if they formed a bond. After copying down the Chemical formula, next, list the unique bonds between pairs of atoms (Example. C-H, O-H, N-H).
2. In column 3, determine the electronegativity differences between each pair of bonded atoms identified.
3. In column 4, write down the classification of each identified bond according to the electronegativity difference from column 3, and **figure 5**.
4. In column 5, determine if the molecule is polar or nonpolar overall (see the discussion over the last three pages [pgs. 12 – 14] for a refresher of molecular polarity).

Data Table 3:

Chemical Formula	Unique Bonds between atoms (ex. C-H, N-H, O-H)	Electronegativity difference for each unique bond (use figure 3) (Example: 1.5 for C-F)	Bond classification (figure 5) Example: C-H is Nonpolar bond C-F is Polar bond	Is it a Polar or Nonpolar Molecule? **Check the net dipole moment.
Example: HCN	C-H C-N	0.4 for C-H 0.5 for C-N	C-H is a Nonpolar bond C-N is a Polar bond	HCN is a POLAR molecule.