Introduction

The purpose of the laboratory exercise is to review Lewis dot structures and expand on topics discussed in class. Additional topics covered are the general shapes and bond angles of different molecular groups. For a detailed discussion of Lewis dot structures review your textbook (Hein Ch 11) and lab Experiment 11 (performed last semester).

Discussion

All atoms are formed of a nucleus containing protons and neutrons surrounded in space by electrons which are held within specific regions of space by the attractive force of the protons. An early theory for predicting the formation, and structure of molecular compounds was formulated by Lewis. The theory says that the outermost electrons in an atom, often referred to as **valence electrons** are involved in bonding atoms together to form compounds. The valence electrons for the representative elements are the sum of the s and p electrons in the outermost shell (largest principle quantum number), and is also the same as the group number on most periodic tables.

Lewis Dot Structures

Lewis electron dot structures or simply **Lewis structures** are a useful construct to keep track of valence electrons in representative elements. In this notation the valence electrons are represented by dots surrounding the atomic symbol of an element. Several examples are shown below in Figure 1. Ions are shown in brackets with the corresponding charge. The formation of ionic compounds will be discussed in lecture.

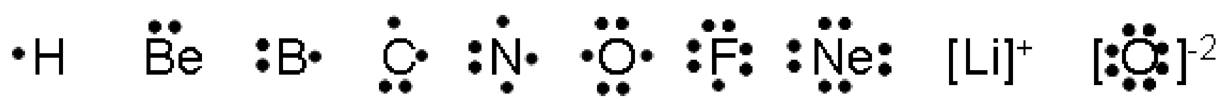


Figure 1: Example Lewis dot structures for several atoms, and ions.

The formation of molecular bonds, and the sharing of electrons is driven by the desire for atoms to achieve the **noble gas configuration**. From quantum mechanics this is represented as having filled orbitals or a s^2p^6 configuration like that of the noble gases. This is often referred to as the **octet rule**, meaning that all atoms (except H and He) want to have 8 electrons in the outermost orbital. Ionic compounds achieve this by cations losing electrons and anions gaining electrons, but molecular compounds are forced to share the electrons in order to achieve octets. The octet rule is only a general guideline, and breaks down when considering d-orbitals, and in several other cases as discussed in lecture and in your book. The most important exception is for hydrogen, which only requires two electrons to achieve a noble gas configuration (He).

A Lewis structure for molecular compounds is a 2D representation in which electrons that are shared between two atoms are represented as a single line connecting the atoms. If multiple pairs of electrons are shared they are represented by multiple lines between the atoms. Unshared or **lone-pair electrons** are represented by dots located around the atom. For polyatomic ion, the rules are the same except that the group of atoms is enclosed in brackets and the overall charge of the ion is shown. Figure 2 shows several examples.

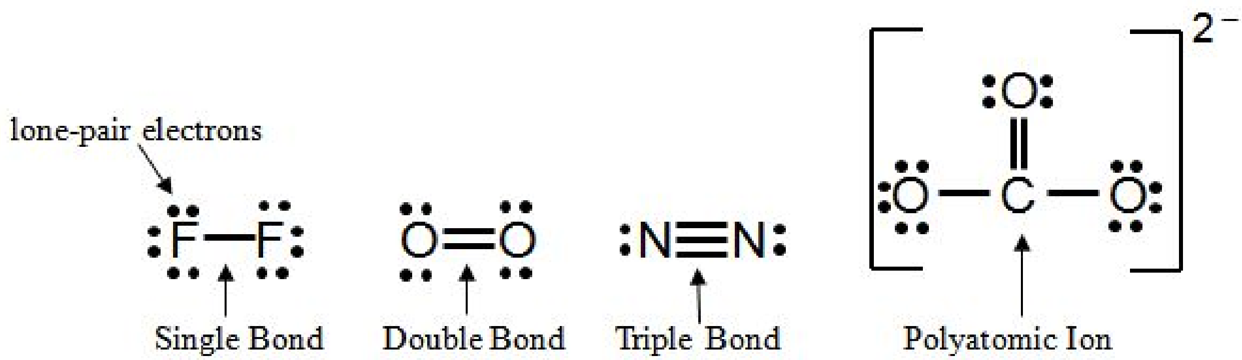


Figure 2: Example Lewis dot structures for several molecules.

Molecular Model Building (3D Models)

The 3D structure of molecules is often difficult to visualize from a 2D Lewis structure. In order to understand the true 3D shape of molecules molecular model kits will be used to create 3D models. This will make it easier to see the common geometric patterns which Lewis theory predicts molecules will form.

Atoms in molecules or polyatomic ions are arranged into geometric shapes which allow the electron pairs to remain as far apart as possible in order to minimize the repulsive forces between them. The underlying theory is call **valence shell electron pair repulsion (VSEPR)** theory. For well behaved molecules that obey the octet rule there are six basic shapes molecules can assume as shown in Table 1.

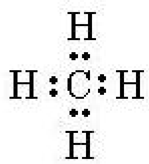
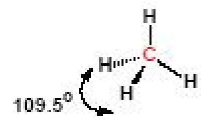
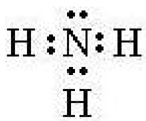
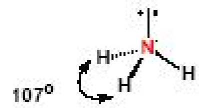
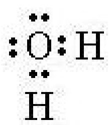
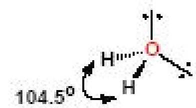
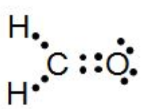
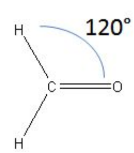
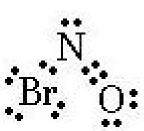
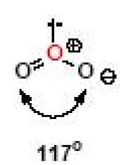
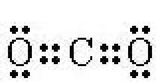
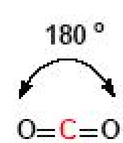
Lewis Structure	# charge clouds	# atoms bonded to	# lone pairs	Molecular Shape	Bond Angle	Molecular Polarity	3D Structure
	4	4	0	Tetrahedral	109.5	Non-polar or Dipolar	
	4	3	1	Trigonal Pyramidal	109.5	Dipolar	
	4	2	2	Bent - 109.5	109.5	Dipolar	
	3	3	0	Trigonal Planar	120	Non-polar or Dipolar	
	3	2	1	Bent - 120	120	Dipolar	
	2	2	0	Linear	180	Non-polar or Dipolar	

Table 1: Six basic shapes for Lewis Structures using s and p electrons only.

Bond angles (Figure 3) always refer to the angle formed between two end atoms with respect to a central atom. If there is no central atom there is no bond angle. The size of the angle depends mainly on the repulsive forces between electron pairs around the central atom. According to VSEPR theory the atoms and electrons around the central atom try to remain as far apart as possible. The bond angles determined are estimates only, and the real bond angles can differ by several degree's depending on the molecule studied.

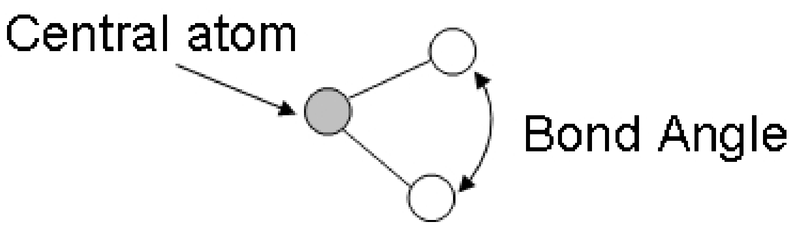


Figure 3: Bond angles.

Bond Polarity

Electrons in molecular compounds are shared between two atoms to form bonds. For atoms that are alike (diatomics) the sharing is equal, but for most other molecules the sharing is unequal. **Electronegativity** is the attractive force an atom has for the shared electrons in a bond. Electronegativity values are assigned to elements, and can be found in Figure 4. In general electronegativity increases as we move across a row, and decreases as we move down a column.

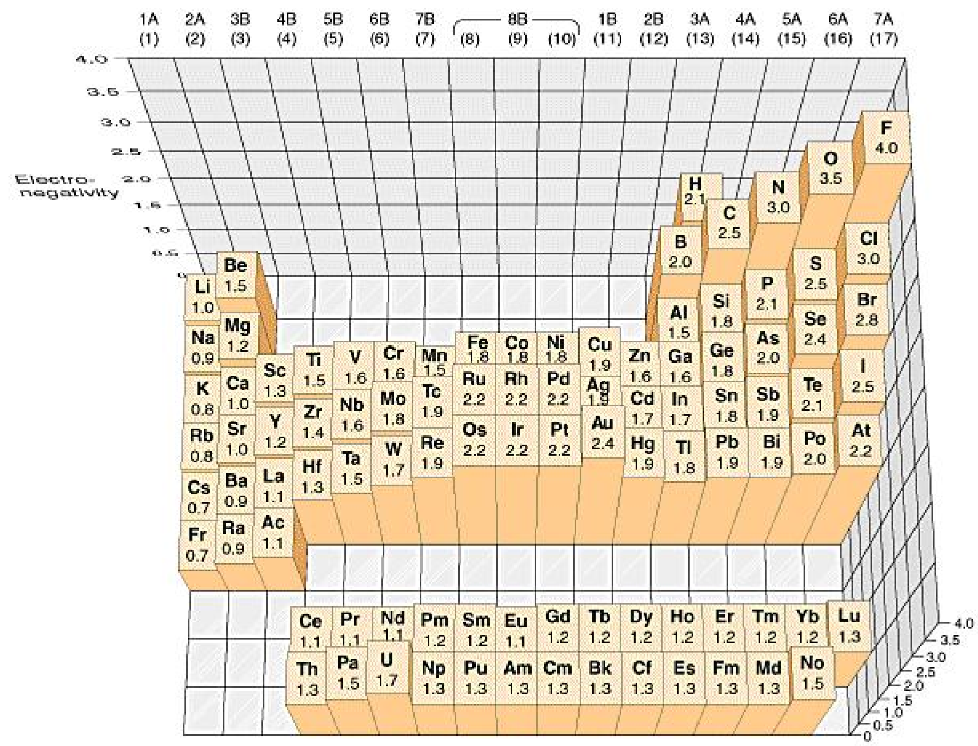


Figure 4: Electronegativity values.

Atoms that share the electrons in a bond equally are called **non-polar covalent bonds or covalent** bonds, while those that are shared unequally are called **polar covalent** bonds. Bond polarity in atoms can be indicated by using the greek symbols $\delta+$ to indicate a small excess of positive charge, or $\delta-$ to indicate a small excess of negative charge from the unequal sharing. Another common method is to use a modified line for the bond with an arrow pointed toward s the more electronegative atom, and a small cross toward s the more electropositive atom. Figure 5 shows an example of each method.

Molecular Dipoles

Just as individual bonds in molecules can be polar and non-polar, molecules as a whole are often polar because of the net sum of individual bond polarities and lone-pair contributions in the molecule. The resulting **molecular dipoles** can be thought of as the center mass of all positive charges being different than the center of mass for all negative charges. Another way of looking at it is a "tug of war" between the positive and negative ends of the polar bonds, if polar bonds tug in opposite

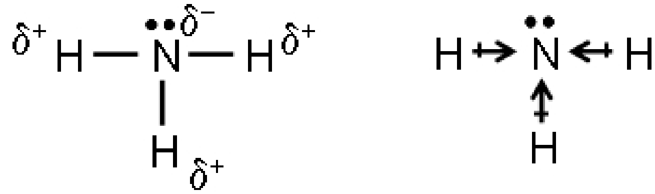


Figure 5: Bond polarity in an ammonium molecule.

directions as shown in Figure 6 then the molecule is considered **nonpolar**, but if the polar bonds align, or do not cancel out then there is a net dipole and we consider the molecule to be **dipolar** as shown in Figure 6.

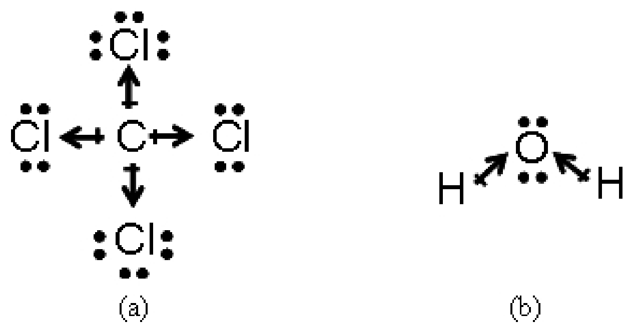


Figure 6: Molecular Dipoles (a) Nonpolar molecule due to symmetry (b) Dipolar molecule.

Drawing Lewis Structures

Drawing Lewis structures takes time and practice, and there is no single set of steps that will always yield the correct answer. Expect to occasionally draw several incorrect models before you find the correct one. Learn from each incorrect model what does and does not work, and apply it to drawing future Lewis structures. The general rules below will generally lead to the correct structure in one or two iterations.

1. Add up the valence electrons
   (a) Add up the valence electrons for all regular atoms (s and p orbitals with the highest quantum number)
   (b) Add electrons for molecules with a negative charge (ex: ${CO_3}^{-2}$)
   (c) Subtract electrons for molecules with a positive charge (ex: ${NH_4}^{+}$)
2. Write a trial structure
   (a) Place the least electronegative atom in the center
   (b) Carbon is generally a central atom and forms bonds with itself frequently
   (c) Make molecules as symmetrical as possible
   (d) Hydrogen has only one valence electron, and can only form one bond and is therefore never the central atom
   (e) Draw one bond between all atoms
   (f) Typical bond numbers formed (H = 1, O = 1 or 2, C = 4, N = 1, 2, or 3)
   (g) Oxygen rarely bonds to another oxygen (except for peroxides), instead forming single or double bonds to other atoms
   (h) F, Cl, Br, and I generally form 1 bond (but not always)
3. Count electrons - Subtract 2 electrons for every bond formed
4. Distribute the remaining electrons to give noble gas configurations (octet rule)
   (a) Surround each atom with 8 electrons (except H)
   (b) Start with the most electronegative atoms first
   (c) If all atoms have 8 electrons around them you are done, if not remove unshared electron pairs from outer atoms and form double and triple bonds

Laboratory 20: Review of Lewis Dot Structures

Name: ______________________ Class: ________________ Date: ________________

1. What is the octet rule?

2. What atom(s) is the exception to the octet rule?

3. Complete the following table. Do not fill in the shaded sections. For the typical structures formed column, draw lewis structures (including lone pair electrons) showing the typical lewis structures that would be formed by the atom in a compound. There is more than one possible structure for many of the atoms. If the structure does not have a shape/bond angle then put N/A in the answer blank.

Element	Number of Valence e^-	Number of Bonds Formed	Typical Structure(s)	Molecular Geometry	Bond Angle
Carbon (4 Answers)					
Hydrogen (1 answer)					
Oxygen (2 answers)					
Nitrogen (3 answers)					
Halogens (1 answer)					

4. How does the table above illustrate the octet rule?

Building 3D Models

Use the ball and stick kits provided in class to build 3D models of the molecules after you have drawn the Lewis structures. The balls are color coded as shown in Table 2.

Ball/Stick	**Use**
Black (4 holes)	Carbon - tetrahedral
Black (3 holes)	Carbon - trigonal planar
Red (2 holes)	Oxygen
Green (1 hole)	Halogens
White (1 hole)	Hydrogen
Light Blue (4 holes)	Nitrogen
Inflexible bonds	Single bonds, and lone pair electrons
Flexible bonds	Double and Triple Bonds

Table 2: Ball and Stick Model Parts.

Molecular Geometry

For each of the molecules listed below:

1. Draw the lewis structure.
2. Build a 3D model, show your instructor the model.
3. Describe the molecular geometry (Tetrahedral, Trigonal Pyramidal, Bent, Trigonal planar, and Linear of the starred atom(s) ($^*X$)
4. Determine the bond angles around the starred atom(s).

Molecule	**Lewis Structure**	**Line Drawing**	**Model**	**Geometry**	**Bond Angle**
$^*CH_4$					
$CH_3(^*CH_2)_3CH_3$					
$CH_3{}^*CH(CH_3)CH_2CH_3$					
$CH_3{}^*CH{=}CHCH_3$					
$CH_3{}^*C{\equiv}CCH_3$					

Molecule	Lewis Structure	Line Drawing	Model	Geometry	Bond Angle
CH_3*CH_2*OH				C: O:	
CH_3*CH(*OH)CH_3				C: O:	
CH_3CH_2*CHO					
CH_3*$COCH_3$					
*CH_3*OCH_3				C: O:	
*CH_3*NH_2				C: N:	
CH_3*$NHCH_3$					
*$N(CH_3)_3$					
*CH_3*CN				C1: C2:	
CH_3CH_2*COOH					
CH_3*CH_2*CO*OCH_3				C1: C2: 02:	

5. When using line drawings molecules are often represented as zig-zag lines. For example: $CH_3(CH_2)_7CH_3$ is generally drawn like: 
Based on your models above why is this the "best" representation?

6. There are two possible structures for the fourth lewis structure ($CH_3-{}^*CH{=}CH-CH_3$). Draw the lewis structure for the other possible structure. Identify the Geometry **AND** Bond angle of the indicated atom.

7. Some types of carbon carbon bonds allow molecules to be rotated freely, while others do not.
Which bond type(s) (C−C, C=C, C≡C) do not allow free rotation?