Chemical Bonds, Lewis Structures, Bond Order, and Formal Charge

PRELAB ASSIGNMENT

Read the entire laboratory write up. Write an objective, any hazards associated with this lab, and answer the following questions in your laboratory notebook before coming to the lab. Read the entire laboratory write up before answering the flowing questions.

1. (a) How many electrons are shared in a single bond?
   (b) How many electrons are shared in a double bond?
   (c) How many electrons are shared in a triple bond?
2. Describe at least two differences between a sigma, σ, and a pi, π, bond.
3. (a) How many sigma bonds help make up a double bond?
   (b) How many sigma bonds help make up a triple bond?
4. What is the difference between lone electron pairs and bond electron pairs?
5. What is the difference between counting the number of bonds and the number of bond electron pairs in a molecule?
6. Briefly explain why electrons occur as pairs.
7. What's the difference between an ionic bond and a covalent bond?
8. How many electrons are generally found around a metal atom in the Lewis structure for an ionic compound?
9. How many electrons are generally found around a non-metal atom (other than H or He) in a Lewis structure?
10. (a) What is bond order and (b) how is bond order calculated?
11. (a) What is formal charge and (b) how is it calculated?

BACKGROUND INFORMATION

A **bond** is the sharing or transfer of electrons between two atoms within a molecule or crystal lattice. The properties of chemical compounds are directly related to the ways in which atoms are bonded together to make molecules or crystals. **Valence electrons**, or an atom's outermost electrons, participate in bond formation. The Group number of a main Group (Group A) element can tell you the number of valence electrons each element has. The chemical bonds that hold atoms together in molecules consist of pairs of electrons (or two electrons) shared or transferred between atoms. Recall that an orbital can contain up to two electrons each with opposite spins. Atoms in a **covalent bond** tend to share valence electrons in such a way that each atom has a share in an octet, or eight, valence electrons. Note that eight valence electrons correspond to full s and p orbitals. A **single bond** consists of two shared or transferred electrons. Single bonds are always **sigma, σ, bonds**. Sigma bonds always lie in the plain of the bonding atom's nuclei and may be formed by overlapping s orbitals, overlapping s and p orbitals or overlapping p_x orbitals oriented head to head. Multiple bonds are composed of two or more different bonds making up one multiple bond. A **double bond** consists of four shared electrons, and a **triple bond** consists of six shared electrons. Double and triple bonds are only formed between two non-metal atoms. Double bonds contain one sigma bond and one **pi, π, bond**. Triple bonds contain one sigma and two pi bonds. Pi bonds lie in the planes above and below (or in front and behind) the plain of the bonding atom's nuclei. Pi bonds are formed by overlapping parallel p_y or p_z orbitals. Hydrogen and most metals cannot form pi bonds because they do not have valence electrons in p orbitals. Electron pairs that are part of a bond are called **bond pairs**. **Lone electron pairs** are pairs of electrons that are not part of a bond.

Lewis structures illustrate the arrangement of valence electrons in molecules and ions. Lewis structures are not accurate representations of ionic compounds because ionic compounds exist as crystal lattices as opposed to single molecules. However, Lewis structures are sometimes used to illustrate the structure of molecules containing ionic bonds. In Lewis structures atoms in an **ionic bond** tend to transfer valence electrons in such a way that metal atoms (or cations) with low ionization energies have no electrons and nonmetal atoms with large negative electron affinity values have a share in an octet, or eight, valence electrons. In Lewis structures atoms in a covalent compound, other than H or He, share valence electrons in such a way that all atoms have a share in an octet, or eight, valence electrons.

To draw Lewis structures

1. Determine which atom will be in the center of the molecule. The element with the least negative electron affinity and lowest ionization energy is generally in the center. Hydrogen is generally on the outside and carbon generally in the center.
2. Note the number of electrons contributed by (the number of valence electrons for) each atom. Then add the electrons contributed by the individual atoms to obtain the total number of valence electrons in the molecule or ion. For ions remember to include the number of electrons the atom has lost or gained.
3. Arrange the outer atoms around the central atom and connect each atom to the central atom with a single (sigma) bond.
4. Subtract the number of electrons involved in sigma bonds from the total number of valence electrons available. Assign the remaining lone pairs of electrons to the elements with the most negative electron affinity first.
5. Check to see that each atom has a share in 8 electrons. If an atom does not have a share in 8 electrons, determine how many electrons the atom needs to complete an octet.
6. Add pi bonds to form double or triple bonds if needed to complete an octet for each atom. Do not form a double or triple bond if a single bond configuration provides an octet for all non-metal atoms.

Some molecules violate the octet rule by containing a nonmetal atom with 7 rather than 8 electrons (or being one electron short of an octet). Such molecules are called **radicals or free radicals** and are highly reactive.

A **bond** is the sharing or transfer of electrons between two atoms within a molecule or crystal. Note that there is one bond between the two bromine atoms in Br—Br and one bond between the two carbon atoms in acetylene, H—C≡C—H. The one bond between the two bromine atoms is a single bond and the one bond between the two carbon atoms is a triple bond. **Bond order** is the number of electron pairs shared between two types of atoms within a molecule. For most bonds the type of bond indicates the bond order. In other words the bond order is 1 for a single bond, 2 for a double bond, and 3 for a triple bond. However, in resonance structures two identical types of atoms may appear to be connected by different types of bonds within an ion or molecule, for example $[O - N = O]^- \leftrightarrow [O = N - O]^-$. When this occurs, the bond order is calculated as the number of electron bond pairs divided by the number of bonds connecting these type of atoms in the ion or molecule, or

$$\text{Bond order} = \frac{\text{number of shared electron pairs in all X-Y bonds}}{\text{number of X-Y bonds in the molecule or ion}},$$

where X and Y represent elements forming bonds.

For $[O - N = O]^{-} \leftrightarrow [O = N - O]^{-}$, there are 3 electron pairs involved in two bonds (one single bond and one double bond).

$$\text{Bond order} = \frac{3}{2} = 1.5$$

Recall that resonance structures are actually hybrids between the different representations shown.

Each atom within a compound or polyatomic ion has a **formal charge**. Formal charge is an accounting system for assigning electrons to atoms within a molecule. Formal charge is not the actual charge of atoms within molecules. The formal charge of an atom is calculated as the group number – [the number of lone pair electrons (LPE) + ½(the number of electrons in bonds (BE)]. Note that in calculating formal charge you are using the number of electrons rather than the number of electron pairs. The sum of the formal charge of each atom in a neutral compound should be zero. The sum of the formal charge of each atom in a polyatomic ion should equal the charge of the ion.

$$\text{Formal charge = group number of the atom} - \tfrac{1}{2}(\text{BE}) - \text{LPE} \quad \text{or}$$

$$\text{Formal charge} = \text{group number of the atom} - [\text{LPE} + \frac{1}{2}(\text{BE})]$$

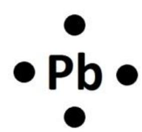
For the polyatomic ion cyanide, $[{:}C{\equiv}N{:}]^{-}$, carbon has a formal charge of 4 – (½)(6) – 2 = **-**1 and nitrogen has a formal charge of 5 – (½)(6) – 2 = 0. Notice that 0-1 = -1 and cyanide has a charge of -1.

PROCEDURE

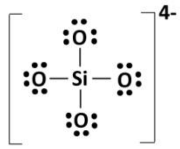
For each atom, ion, or molecule in the tables below:

(1) Determine the total number of valence electrons, and
(2) Draw the Lewis structure following the steps listed previously.

The elements in the following table are either natural components of air or are air pollutants. Complete the number of valence electrons and Lewis structure for each element. The element lead is completed as an example.

Element	Total valence electrons	Lewis structure
Lead, Pb	4	
Nitrogen, N		
Oxygen, O		
Argon, Ar		

Complete (1) the number of valence electrons, (2) Lewis structure, (3) bond order for each type of bond, and (4) the formal charge for each atom in the ion in the table below. The silicate ion, SiO_4^{4-} is completed for you as an illustration. Notice that brackets are placed around the Lewis structure of ions with the charge as a superscript to indicate that the structure is an ion rather than an atom or molecule. Please **DO NOT** look up structures on the web and copy those structures onto this sheet. Please complete this sheet first and check your answers with your e-book. Be cautious of web sources. You might find the following websites useful: http://www.chem.ucla.edu/harding/lewisdots.html, and http://chemwiki.ucdavis.edu/Core/Theoretical_Chemistry/Chemical_Bonding/Lewis_Theory_of_Bonding/Lewis_Structures.

Ion	Total valence electrons	Lewis structure	Bond order for each type of bond	Formal charge for each atom
Silicate, SiO_4^{4-}	32		Si-O → 1	Si → 0 O→ -1
Chloride, Cl^-			NA	NA
Oxide, O^{2-}			NA	NA
Nitride, N^{3-}			NA	NA
Nitrate, NO_3^-				
Carbonate, CO_3^{2-}				
Potassium, K^+			NA	NA
Calcium, Ca^{2+}			NA	NA

Ammonium, NH_4^+				

Most of the following compounds are either natural components of air or air pollutants. Complete (1) the number of valence electrons, (2) the Lewis structure, (3) the bond order for each type of bond, and (4) the formal charge for each atom of the molecules in the table below.

Molecule	Total valence electrons	Lewis structure	Bond order for each type of bond	Formal charge for each atom
Oxygen, O_2				
Ozone, O_3				
Nitrogen, N_2				
Nitrogen monoxide, NO (this is a free radical)				
Nitrogen dioxide NO_2 (this is a free radical)				
Carbon monoxide CO				
Carbon dioxide CO_2				

Sulfur dioxide SO_2				
Sulfur trioxide SO_3				
Water H_2O				
Ammonia NH_3				
Carbonic Acid H_2CO_3 (you've already drawn the structure of carbonate)			C-O $\rightarrow$ H-O $\rightarrow$	
Nitric Acid HNO_3 (you've already drawn the structure of nitrate)				
CCl_3F a Chlorofluorocarbon or CFC (C is central)			C-Cl $\rightarrow$ C-F $\rightarrow$	
CCl_2F_2 a Chlorofluorocarbon or CFC				

$CClF_3$ a Chlorofluorocarbon or CFC				

QUESTIONS

Answer all questions in your laboratory notebook.

1. Based on their Lewis structures why do you think argon atoms exist for long periods of time in nature as a single atom while oxygen and nitrogen atoms do not?

2. Nitrogen monoxide and nitrogen dioxide, components of photochemical smog, are highly reactive compounds that are toxic to plants and animals. Based on their Lewis structures, why do you think they are so reactive?

3. Based on their Lewis structures explain why polyatomic ions exist as stable entities in aqueous solution?

4. What trends do you see in the Lewis dot structures for molecules having the same number of total electrons and the same number of atoms in their structures?

5. Do you see any trends or patterns between the bond order for resonance bonds and the number of resonance structures possible for the compound? If so please describe the trend or pattern you observed.