Learning Objectives and Worksheet VI

Chemistry 1B-AL Fall 2016

~~Lectures~~ (10-12) "Classical" Theories of Molecular Structure and Geometry (Part 1)

Read pp. 621-650 and 602-606 *[back to molecular polarity dipole moments]*
Supplementary video: Orbitals: Crash Course Chemistry http://youtu.be/cPDptc0wUYI

The next three class sessions will be devoted to asking two questions: i) how do atoms combine in forming covalent bonds in polyatomic molecules and ii) what geometries do the atoms assume in three-dimensional space. In this first look at polyatomic molecules we will again take a 'classical' approach: bonding will be considered in the context of Lewis octet configurations (Lewis dot structures) and most stable geometries will be determined by electrostatic interactions. These approaches are very useful and the results will be consistent with the quantum mechanical description that we will study in future sessions.

I. Lewis molecular structures

1. Obtain structure where:
   i. Number of electrons shown in structure is equal to the total number of valence electrons in the constituent atoms or ions
   ii. By virtue of shared electrons or non-bonding pairs each atom has a complete shell (2-electron duet for H-atoms, and 8-electron octet for second, and higher, row atoms)
2. Zumdahl (p. 623) OR
3. **L**ewis **V**alence **E**lectron **D**iagrams **(LVEDs)**
   i. the LVEDs for second and third row atoms are:

H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar

ii. Applying the LVEDs for 'common motifs' of bonding

a. hydrogen shares _____ pair of electrons forming _____ covalent bond.

b. carbon shares _____ of electrons forming _____ covalent bonds.

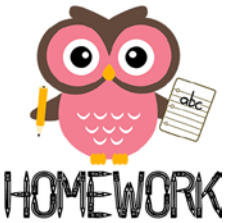
c. nitrogen forms _____ covalent bonds and has _____ non-bonding pair.

d. oxygen forms _____ covalent bonds and has _____ non-bonding pairs.

e. fluorine forms _____ covalent bond and has _____ non-bonding pairs.

f. In some molecules containing a negatively charges O^- atom, the O^- will form _____ covalent bond and have _____ non-bonding pairs.

4. Multiple Covalent Bonds: To obtain an octet, two atoms may share more than one pair of electrons.



HW#5: **36**

i. Common motifs are double bonds where two atoms share _____ electrons and triple bonds where two atoms share _____ electrons.

ii. In comparing the properties of single and multiple bonds what is generally true in regard to their:
bond strengths (bond energies):
bond lengths:
bond order:

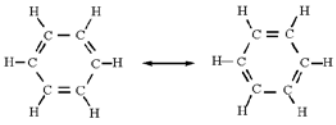
5. To become facile with drawing Lewis structures you must:

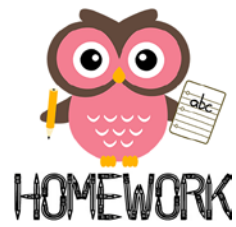
_____, _____, _____ !!!!

II. Resonance Structures

1. All resonance structures of a molecule have identical stoichiometric formulas; all isomeric structures of a molecule have identical stoichiometric formulas. What is the distinction between the meaning of different resonance structures and different isomeric structures ?

2. What experimentally measured property would distinguish between C_6H_6 existing as a mixture of the two structures below and as a resonance hybrid of the structures?





HW#5: **37,38, S9****

III. Formal charge

1. Formal is concept for assigning net charges to the atoms in a molecule. I first "strips" off the valence electrons leaving positively charges atomic centers and then returns negatively charged valence electrons to the various atoms.
2. For the following atoms what would be their 'starting' positive charge contribution to the formal charge on the atom:
   i. B +____
   ii. N +____
   iii. F +____
   iv. O +____
   v. H +____
3. The negative charges 'valence' electrons are then distributed among the atoms with the following conventions:
4. A non-bonding pair of electrons is assigned to _____ making a contribution of – ____ to that atom's formal charge.
   i. For each pair of electrons by two atoms, the assignment is _____ making a contribution of – ____ to each atoms formal charge.
   ii. The sum of formal charges must _____ to the _____ on the molecule or molecular ion.
5. We saw that when a molecule has two "equivalent" octet structures, the resulting resonance hybrid is an average structure with equal contributions from the two Lewis structures. More generally, if there are several, but non-equivalent, octet structures that can be drawn for a given molecule, the resulting hybrid will be a weighted average of the possible octet structures. What three factors will determine the best Lewis structures, i.e. the Lewis structures that will dominate (contribute most strongly) to the weighted average hybrid?

HW#5: **39, 40, S10**

IV. Non-octet Lewis structures

1. Third row and higher atoms may have structures where in a molecule the atom may have a shell with _____, _____, _____, or _____ electrons being shared or as non-bonding electron pairs.
2. This occurs in atoms of third row and higher because of the "availability" of _____ that can participate in bonding.
3. Although it may be possible to construct both octet and non-octet structures for a given molecule or ion, the non-octet structures are often preferred (i.e. make a greater contribution to the actual structure) since the will have more favorable _____.

A toolkit for constructing and testing yourself on Lewis dot structures:

http://www.stolaf.edu/depts/chemistry/courses/toolkits/123/js/lewis/

Lewis dot tutorials:

https://chemistry.boisestate.edu/richardbanks/inorganic/electron-dot.htm