Learning Objectives and Worksheet IX

Chemistry 1B-AL Fall 2016

Sessions ~~Lectures~~ (15-16) Bonding in Polyatomic Molecules:

RETURNING TO THE FIRST PART OF CHAPTER 14 (pp. 633-676), to cover covalent bonding in polyatomic molecules, and then onto molecular dipoles (pp 688-692).

In the previous class sessions we have investigated how covalent bonds are formed by the constructive interference of atomic orbitals on two atoms in a diatomic molecule. Now we are prepared to extend these concepts to polyatomic molecules.

I. Ground state atomic configurations do not predict molecular structures

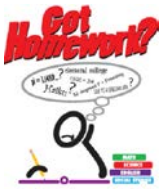
1. In the H_2 molecule we saw how atomic orbitals containing an unpaired electron on each H atom interact to form a bonding molecular orbital that accommodated the electron-pair. For the atoms below, indicate the formulas of the hydrides that would be formed by an H· atom combining with unpaired electrons in the atom's ground state to form X–H bonds.
   i. Li
   ii. Be
   iii. B
   iv. C
   v. N

2. In the ground state of atomic nitrogen, $1s^2 2s^2 2p_x 2p_y 2p_z$ ↑ ↑ ↑, 3 H· atoms could interact with the unpaired electrons in the 2p orbitals to form the stable octet structure NH_3. From your knowledge of the geometry of the $2p_x$, $2p_y$, and $2p_z$ atomic orbitals the predicted H–N–H bond angle would be _____ **°.**

II. General principles of hybridization

1. In forming covalent bonds in polyatomic molecules hybrid orbitals may be utilized. A hybrid orbital consists of _____ that may include both occupied and unoccupied in the atom's ground state configuration.

2. In forming hybrids what are the "costs" in terms of energetics (i.e. higher energy relative to atom): _____ would be a cost of forming hybrids. This is why isolated atoms do not "naturally" go to a hybridized state.

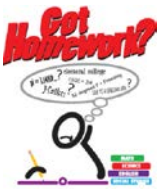


HW#7: **S14**

3. There are several energetic advantages accrued (lowering of energy) when an atom utilizes hybrids to form covalent bonds in a polyatomic molecule. These include:
   i. _____
   ii. _____
   _____
   iii. _____
4. We will see that whether a molecular structure involves primarily atomic or hybrid orbitals depends on the "winner" of the energy costs vs energy gains. In describing the m.o. of diatomic molecules we focused on combinations of unhybridized atomic orbitals. However s-p mixing or sp hybridization was invoked for the energy ordering for B_2, C_2, N_2 but not O_2 or F_2. In terms of energy costs vs gains, why would s-p mixing occur for the lower atomic number 2^{nd} row atoms but not for Z=8 or 9 ?

5. A bonding orbital between a hybrid orbital on boron atom and a H· atom is formed by _____ between the hybrid orbital and a 1s a.o. on the H· atom.

III. sp hybridization



HW#7: **51**

1. In sp hybridization the 2s, $2p_x$, $2p_y$, and $2p_z$ a.o. form _____ sp hybrids leaving _____ unhybridized 2p orbitals.
2. The sp hybrids are directed _____° apart and the unhybridized 2p a.o.'s are _____ to the direction of the sp hybrids.
3. If H· atoms bond with unpaired electrons **in the sp hybrids** the resulting molecular geometry is _____.

Bonding in acetylene C_2H_2 applet (helps with HW#7, 51):
http://switkes.chemistry.ucsc.edu/teaching/Jmol/AcetyleneBonding/AcetyleneBonding.html

IV. sp^2 hybridization

1. In sp^2 hybridization the 2s, $2p_x$, $2p_y$, and $2p_z$ a.o. form _____ sp^2 hybrids leaving _____ unhybridized 2p orbital.
2. The sp^2 hybrids are directed _____° apart and the unhybridized 2p a.o. is _____ to the plane of the sp^2 hybrids.
3. If H· atoms bond with unpaired electrons **in the sp^2 hybrids** the resulting molecular geometry is _____.

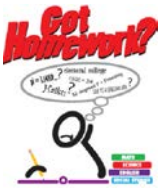
V. sp^3 hybridization

1. In sp^3 hybridization the 2s, $2p_x$, $2p_y$, and $2p_z$ a.o. form _____ sp^3 hybrids leaving _____ unhybridized 2p orbitals.
2. The sp^3 hybrids are directed _____° apart.
3. If H· atoms bond with unpaired electrons **in the sp^3 hybrids** the resulting molecular geometry is _____.

Excellent website to visualize sp3 hybrids:
http://www.uwosh.edu/faculty_staff/gutow/Orbitals/N/sp3%20hybrid.shtml

VI. Bonding in molecules with more than one 2nd row atom

1. In the molecule n-propane $CH_3CH_2CH_3$
   i. the geometry around the central carbon would be _____.
   ii. the C–C bonds would be the result of constructive interference between _____.
   iii. the C–H bonds would be the result of constructive interference between _____.
2. In the molecule propene CH_2CHCH_3
   i. the geometry around the central carbon would be _____.
   ii. the C=C bond[s] would be the result of constructive interference between
   a. _____ and _____ (for one component of double bond)
   b. _____ and _____ (for the second component).
   iii. the C–C single bond would be the result of constructive interference between _____ .



HW#7: **51,54, S15**

VII. When might an atomic bond with unhybridized a.o.'s?

1. The geometry of some molecules with third row central-atoms indicates that the atom is forming bonds with predominantly unhybridized a.o.'s. Why might this be so in terms of the costs and advantages of hybridization?

2. For 'terminal' atoms, that bond to only one additional atom, one cannot use molecular geometry to ascertain the hybridization around the atom. As discussed in class differing textbooks make differing assumptions and the actual results, from quantum mechanical calculations, are often somewhere in between, i.e. partially hybridized. From the class presentation, you should retain our 'agreements' on ambiguous cases:

   i. O in ---X=O _____

   ii. N in ---X-C≡N _____

   iii. ---F,--- Cl,-- O^- _____

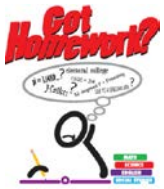
   iv. diatomics _____

Hybrid vs. no hybrid bonding in molecules visualization applet:

http://switkes.chemistry.ucsc.edu/teaching/CHEM1B/WWW_other_links/HybridvsNoHybrid.html

VIII. Dipole moments in polyatomic molecules and delocalized bonding

1. What are two requirements for a polyatomic molecule to have a non-zero dipole moment



HW#7: 52

   i.

   ii.

2. Delocalized bonding most often occurs when p-π a.o.'s interact to form m.o.'s that extend over several atoms in a molecule. These delocalized m.o.'s are often the description of the actual molecule that has several Lewis _____.