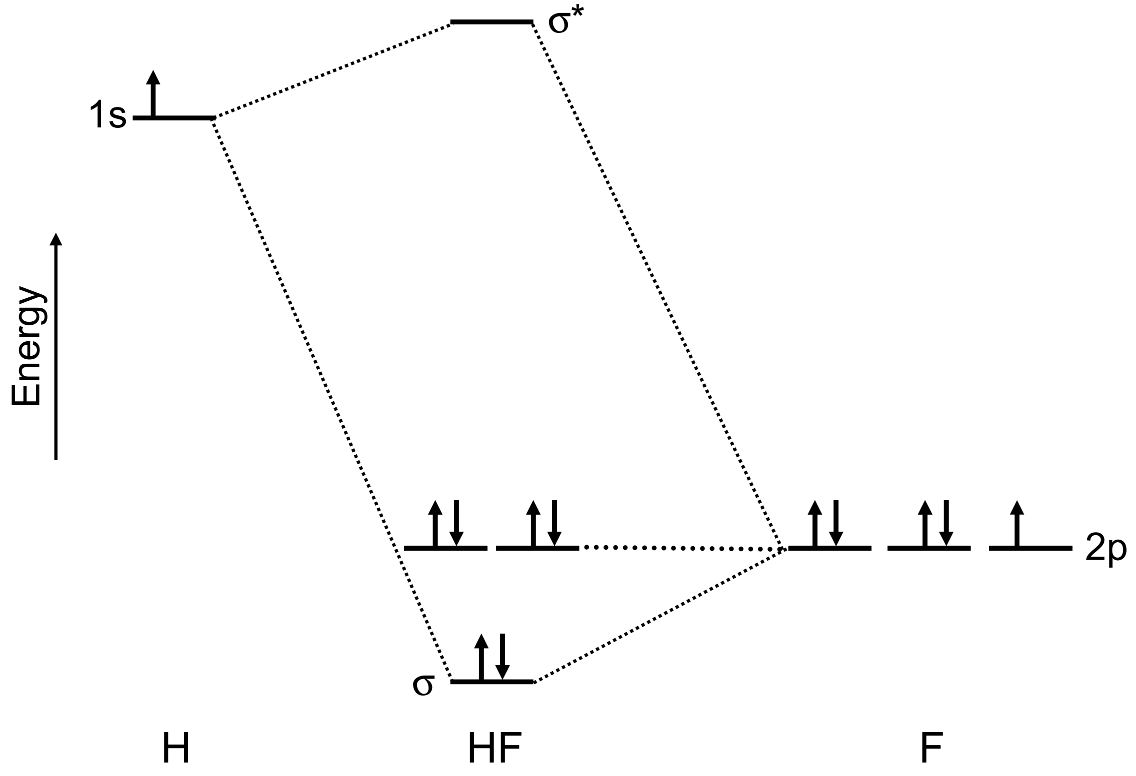
CHEM 121
Spring 2006
Quiz 4

Name: ____

The partial molecular orbital diagram of HF is shown below. The F 2s orbital is not shown because it is much lower in energy than the F 2p orbitals.



1. (5 Points) Fill in the diagram. Remember that the F 2s orbital is not included!

2. (1 Point) The molecular orbitals that result because two F 2p orbitals do not interact with the H 1s orbital are classified as **non-bonding** molecular orbitals. Note that these are the pair between the ones labeled σ and σ*.

3. (1 Points) Which orbital is the LUMO? **The σ* is the LUMO.**

4. (3 Points) What is the bond order in HF? Hint: see question 2.

There are 2 electrons in bonding MOs and no electrons in antibonding MOs (the non-bonding MOs do not count). Therefore, the bond order is 1.

Continued on reverse →

5. (4 Points) Explain why the F orbitals are drawn as having lower energy than the H orbital.

F has a higher ionization energy than H (*because it is farther to the right on the periodic table***). This means that it takes more energy to remove an electron from F than H, which implies that the F orbitals must be lower in energy than those of H.**

6. (4 Points) The F 2s orbital is a valence orbital for F, but only plays a small role in bonding. Explain why.

In MO theory the interaction between two orbitals depends inversely on their energy (*the larger the difference, the smaller the interaction***). Since the F 2s orbital is much lower in energy than the F 2p and the H 1s, its interaction with these orbitals is very small. And thus, it plays only a small role in bonding.**

The F 2s electrons are much more core-like than the F 2p electrons (even though they are still valence electrons) and will be pulled closer to the nucleus. This will result in poorer overlap between the F 2s and the H 1s and lead to a weaker interaction between these orbitals.

7. (4 Points) HF and HCl are expected to have very similar bonding (i. e., their energy level diagrams are almost identical). However, HF is a weak acid and HCl is a strong acid in water. Explain using MO theory. Hint: remember the definition of acid strength.

The Cl atomic orbitals are larger than the F atomic orbitals. Therefore, the overlap of the Cl atomic orbitals with the H 1s will be worse than with the F atomic orbitals and the H-Cl bond will be weaker than the H-F bond. It will, thus, be easier to break the H-Cl bond than the H-F bond to liberate H^+ and H-Cl should be a stronger acid.

Note that this is an oversimplification of the why HF is a weak acid. Remember that acid strength is described by K_a*, which is just another way of writing* ΔG *for the dissociation of the acid. But,* ΔG *for a process depends on both the starting state (HF(aq)) and the ending state (*$H^+(aq) + F^-(aq)$*). In the answer above, we focused only on the starting state and assumed that the ending states for both HF and HCl are the same. This is not necessarily true, as we will see later.*

8. (10 Points) Please attach problem 6-34 to this sheet.

The given K is a K_c *because its units are those of concentration. Therefore, we will work the problem in units of concentration.*

Determine the $[CO_2]$ *initially.*

$$\frac{2.0\ \text{mole}}{5.0\ \text{L}} = 0.40\ \text{M}$$

Set up the ICE table.

	$2\ CO_2\ (g)$	$\leftrightharpoons$	$2\ CO\ (g)$ +	$O_2\ (g)$
Initial	**0.40**		**0**	**0**
Change	**-2x**		**+2x**	**+x**
Equilibrium	**0.40-2x**		**2x**	**x**

Write K for the reaction and substitute the values from the table into this expression.

$$K = \frac{[CO]^2[O_2]}{[CO_2]^2} = \frac{(2x)^2(x)}{(0.40 - 2x)^2} = 2.0x10^{-6}$$

Since K is small, we know that this reaction will not go very far toward products, which means that x is very small.

Assume that x <<0.40.

$$\frac{(4x^2)(x)}{(0.40)^2} = \frac{4x^3}{(0.40)^2} = 2.0x10^{-6}$$

$$x^3 = \frac{(2.0x10^{-6})(0.16)}{4} = 8.0x10^{-8}$$

$$x = 4.3x10^{-3}$$

Check by inspection that $4.3x10^{-3}$ is less than 0.40 *(the first significant figure in $4.3x10^{-3}$ occurs after the last significant figure in 0.40).*

The final concentrations are $[CO_2]$ = 0.39 M, $[CO]$ = $8.6x10^{-3}$ M and $[O_2]$ = $4.3x10^{-3}$ M.

If you used your calculator to solve this problem, then you may have gotten a slightly different answer.