Chemistry 2000 Fall 2017 Test 1 Version B Solutions

1. (a) See figure 1.

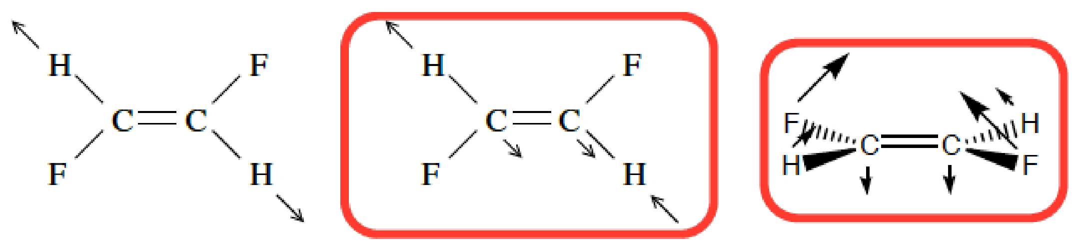
   (b) See figure 1.

   (c) 2p

   (d) The carbon atom uses the two p orbitals in the plane of the molecule to make σ bonds, leaving the p orbital perpendicular to this plane (p_z) available for bonding. The oxygen atom also has a free p orbital perpendicular to the plane of the molecule. The π bond is made by overlapping the p_z orbitals from the two atoms.

2. (a) Trans-1,2-difluoroethene has $N = 6$ atoms. Since this molecule is nonlinear, it has $3N - 6 = 12$ normal modes.

   (b) At equilibrium, difluoroethene has a zero dipole moment because diagonally opposite bond dipoles cancel. Any motion that breaks this diagonal symmetry results in a dipole moment that changes from zero, and therefore makes the mode IR active.



3. (a) HOMO

   (b) The HOMO is entirely localized on the oxygen. Thus, a metal ion (or any Lewis acid) would bind there.

   (c) HOMO: π^{nb}

   LUMO: σ^*

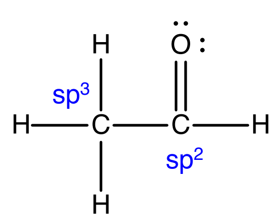


Figure 1: Ethanal with lone pairs and hybridization states

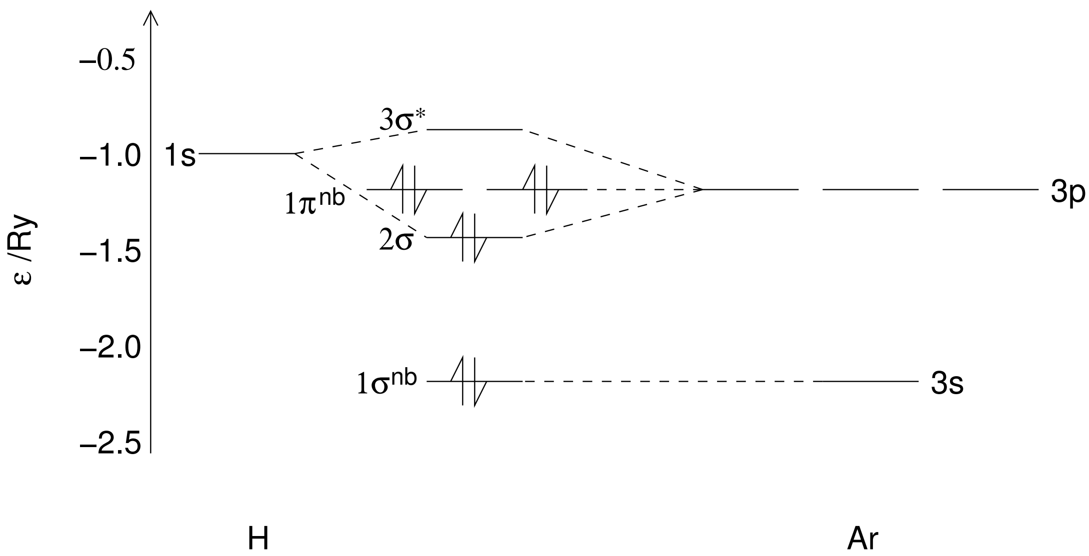
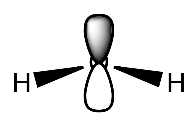
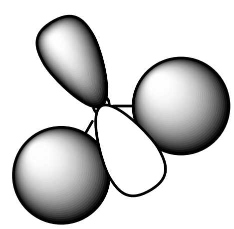


Figure 2: MO diagram of ArH^+.

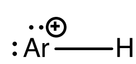
(d) The π^{nb} orbital is just an oxygen p_z orbital:



The σ^* orbital results from combining the H(1s) orbitals with a carbon 2p oriented as shown below:



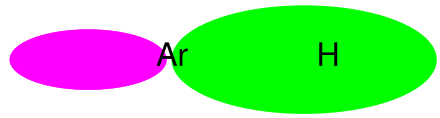
4. (a) Formal charge of argon $= 8 - 6 - \frac{1}{2}(2) = +1$.



(b) See figure 2 for the MO diagram. Bond order $= \frac{1}{2}(2 - 0) = 1$.

(c)
- Both show three lone pairs on the argon atom.
- Both predict a bond order of 1.

(d) The 2σ orbital is obtained by taking a linear combination of the hydrogen 1s and the argon $2p_z$:



(e) ArH would have one more electron, which would end up in the $3\sigma^*$ MO. This would decrease the bond order to $\frac{1}{2}$, but would still form a stable molecule. From what we learned in Chem 1000, we would not be able to explain this non-octet compound. We would in fact be tempted to predict that such a thing could not be made, particularly since the noble gases tend to be unreactive, except with very electronegative elements like fluorine and oxygen. As it turns out however, ArH can be made and has been studied in the gas phase.

5. In a crystal containing N atoms, we would form a 4s band with N states given that each potassium atom contributes one 4s orbital. Each potassium atom has one valence electron, and since each state can hold two electrons, the band would be half-filled. Accordingly, there are many states available near the Fermi level.