Chemistry 2000 Fall 2017 Test 1 Version A Solutions

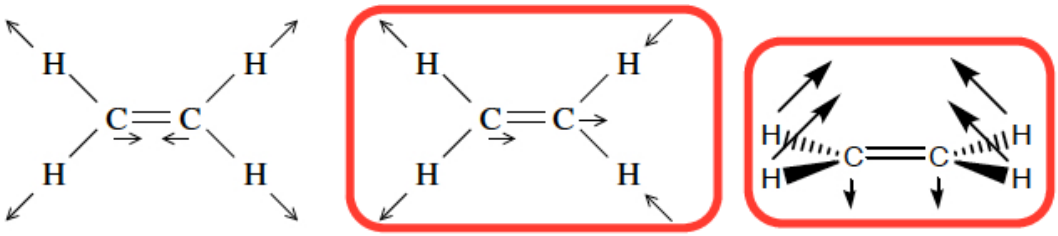
1. (a) See figure 1.

   (b) See figure 1.

   (c) Each carbon atom has one p orbital perpendicular to the molecular plane, conventionally denoted p_z. The p_z orbitals from each atom are overlapped to make the π bond.

2. (a) Ethene has $N = 6$ atoms. Since ethene is nonlinear, it has $3N - 6 = 12$ normal modes.

   (b) Any motions that break the symmetry of the molecule will result in the dipole moment changing from zero during the motion:



3. (a) HOMO

   (b) The HOMO has more electron density at the carbon (based on its size), so a proton should attach there.

   (c) HOMO: σ (bonding)

   LUMO: π^* (for clarity: the asterisk indicates an antibonding orbital)

   (d) For the σ orbital, we combine the p_z orbitals from the two atoms in phase:

   For the π^* orbital, we combine either the p_x or p_y atomic orbitals out of phase:

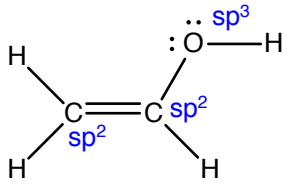


Figure 1: Ethenol with lone pairs, and hybridization states indicated

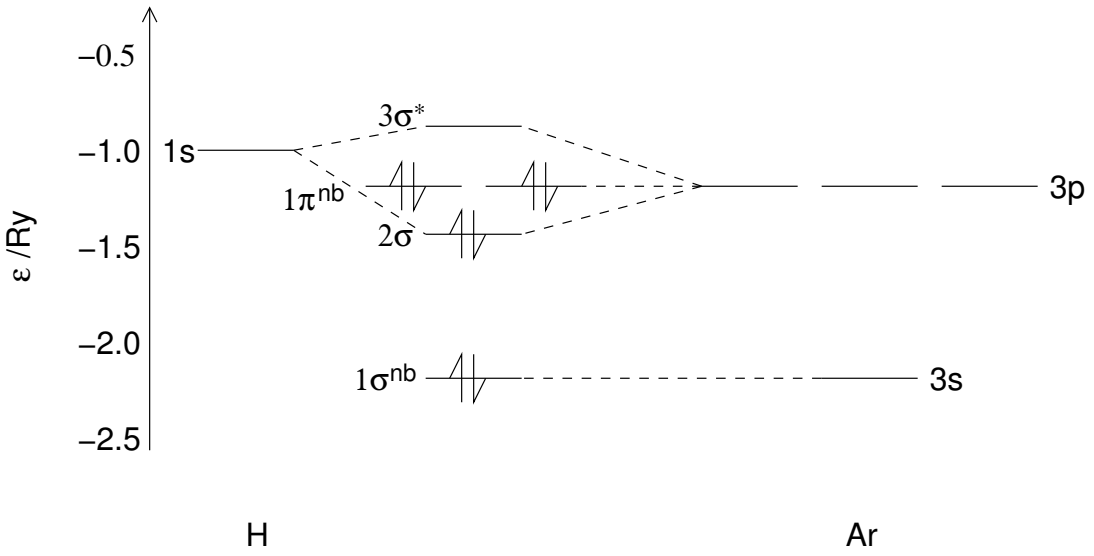
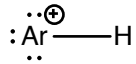


Figure 2: MO diagram of ArH^+.

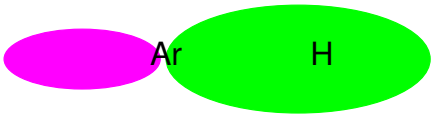
4. (a) Formal charge of argon $= 8 - 6 - \frac{1}{2}(2) = +1$.



(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 2s band with N states given that each lithium atom contributes one 2s orbital. Each lithium 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.