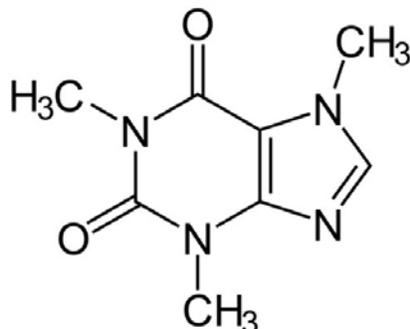
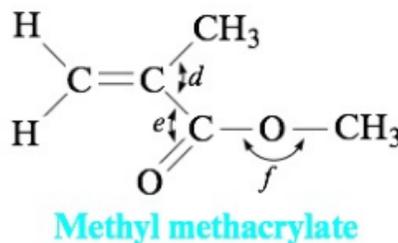
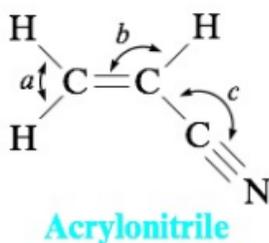


**CHEM 101A Chapter 9 Hybrid and Molecular Orbitals**

1. The structure of caffeine is below. Place lone pairs on any atom to satisfy the octet.. Identify the hybridization of each atom (except hydrogen). Indicate the total number of pi and sigma bonds.

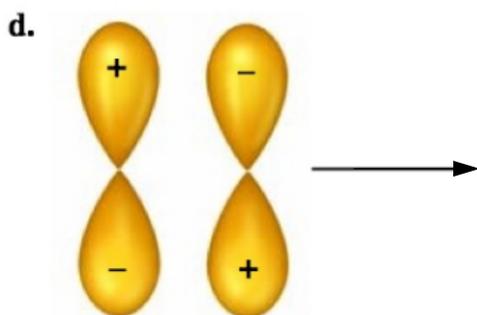
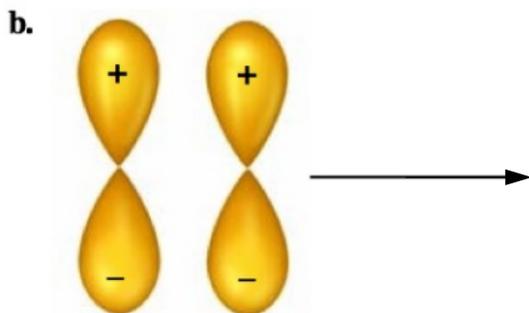
# of  $\pi$  bonds \_\_\_\_\_# of  $\sigma$  bonds \_\_\_\_\_

2. Many important compounds in the chemical industry are derivatives of ethylene ( $C_2H_4$ ). Two of them are acrylonitrile and methyl methacrylate.

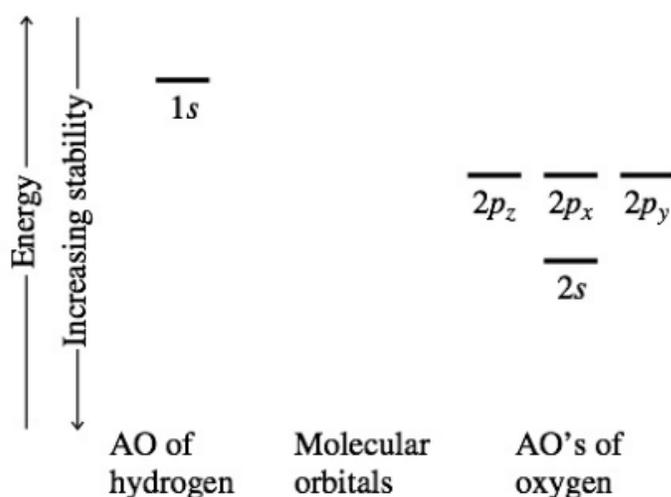


Complete the Lewis structures, showing all lone pairs. Give approximate values for bond angles *a* through *f*. Give the hybridization of all carbon atoms. In acrylonitrile, how many of the atoms in the molecule must lie in the same plane? How many  $\sigma$  bonds and how many  $\pi$  bonds are there in methyl methacrylate and acrylonitrile?

3. Sketch the molecular orbital and label its type ( $\sigma$  or  $\pi$ ; bonding or antibonding) that would be formed when the following atomic orbitals overlap. Explain your labels.



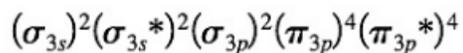
4. The diatomic molecule OH exists in the gas phase. OH plays an important part in combustion reactions and is a reactive oxidizing agent in polluted air. The bond length and bond energy have been measured to be 97.06 pm and 424.7 kJ/mol, respectively. Assume that the OH molecule is analogous to the HF molecule discussed in the chapter and that the MOs result from the overlap of a  $p_z$  orbital from oxygen and the  $1s$  orbital of hydrogen (the O—H bond lies along the  $z$  axis).
- Draw pictures of the sigma bonding and antibonding molecular orbitals in OH.
  - Which of the two MOs has the greater hydrogen  $1s$  character?
  - Can the  $2p_x$  orbital of oxygen form MOs with the  $1s$  orbital of hydrogen? Explain.
  - Knowing that only the  $2p$  orbitals of oxygen interact significantly with the  $1s$  orbital of hydrogen, complete the MO energy-level diagram for OH. Place the correct number of electrons in the energy levels.



- Estimate the bond order for OH.
- Predict whether the bond order of  $\text{OH}^+$  is greater than, less than, or the same as that of OH. Explain.

5. Acetylene ( $\text{C}_2\text{H}_2$ ) can be produced from the reaction of calcium carbide ( $\text{CaC}_2$ ) with water. Use both the localized electron and molecular orbital models to describe the bonding in the acetylide anion ( $\text{C}_2^{2-}$ ).

6. Consider the following electron configuration:



Give four species that, in theory, would have this electron configuration.

7. Which charge(s) for the  $\text{N}_2$  molecule would give a bond order of 2.5?