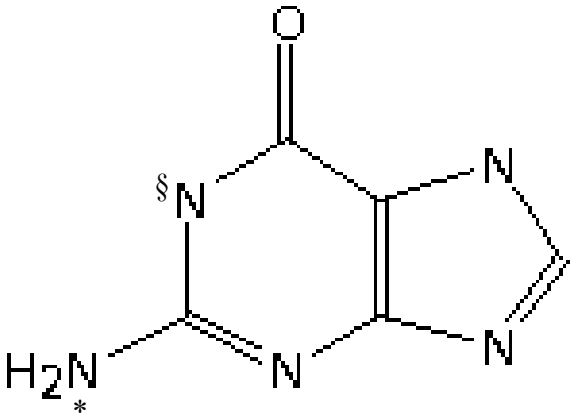
Discussion – 12/13/10
MO Theory and Hybridization

1. Molecular orbitals of CN^-
   a. Draw the Lewis structure of CN^- below, then sketch and label its MO diagram with electrons. Be sure to draw the MOs at the appropriate energies (heights) with respect to C and N. Calculate the bond order for the molecule.

   b. Describe how the Lewis structure is and is not consistent with the MO diagram for the molecule.

   c. Sketch the shapes of the molecular orbitals for CN^- below.

2. Shown below is a shorthand representation of the DNA base, guanine, $C_5N_5OH_5$. The structure has double bonds and single bonds as shown, and as we have seen before, whenever two or more lines come together, there is understood to be a carbon atom.



a. Complete the structure by explicitly writing in the "C" for the carbon atoms, adding hydrogen atoms as necessary, and drawing in lone pairs that are not shown.

b. How many sigma and pi bonds in the molecule?

c. Give the hybridization and bond angles for each of the five carbon atoms in the structure.

d. Give the hybridization and bond angles based on the steric number ALONE for each of the four nitrogens in the two rings, and the N* coming off the ring.

e. i. First, draw the six membered ring structure that is characteristic of the benzene molecule (C_6H_6) that you made in lab. Show the resonance structure that explains how the C-C bonds are all equal length. What are the hybridizations and bond angles for all the carbons? Is the molecule planar? (Note: You have seen this before and should be able to reproduce it on your own.)

ii. Next, redraw JUST the six membered ring of the guanine molecule on the previous page. Indicate the bond angle at each of the 6 atoms in the ring based on steric number alone. Do you see any problem with this structure? Based on your answers to c and d, would you predict that the hydrogen atom bonded to the $N^{\S}$ lies in the same plane as the atoms in the ring? Explain.

iii. Finally, experimental measurements show that all the bond angles in the ring are 120° and the six atoms in the ring and the H bonded to the $N^{\S}$ ARE in a plane. What does this imply about the hybridization of all the atoms in the ring (remember benzene)? Can you draw a resonance structure for guanine that would be consistent with this geometry?