HW #10

assigned: April 6
due: April 13

1. What atomic charges are consistent with the dipole moment of 1.82 Debye of HF?

2. Using mathcad solve for the Hückel MO energies and eigenvectors for the π electrons of ethylene, butadiene, and hexatriene, as well as benzene.

   a) How much is butadiene stabilized by conjugation?

   b) Plot the HOMO-LUMO gap vs. chain length.

   c) According to the Hückel model how much more stable is benzene than hexattiene?

3. Pyridine differs from benzene in that one of the CH's is replaced by N. Suppose that this chemical substitution can be modeled by replacing one of the α's by $\alpha - 0.5$. How does this change impact the energies of the MO's?

What happens as you progress to pyrazine (N's in the "1" and "4" positions to triazine (N's in the "1", "3", "5" positions?

4. Use symmetry to block diagonalize the Huckel Hamiltonian of benzene. Use two symmetry operations. Show that you get the same eigenvalues as obtained with mathcad.

5. Use the CaCHE program to do PM3 calculations on H_2O at HOH angles of 180, 165, 150, 135, 120, 105°.
Use these results to plot the orbital energies vs the HOH angle.

Based on these results would you expect. H_2O^- to be more or less bent than H_2O?