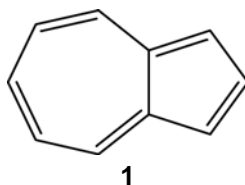


Chemistry 5.04 (F04)
Problem Set 3

Due Friday, 1 October

1. Determine Huckel MO diagram for the two $C_{10}H_{10}$ systems, naphthalene and azulene. Construct the MO diagram of azulene. Compare the resonance energy and bond order of this $C_{10}H_{10}$ system, to that of naphthalene (worked out in Cotton, p 172). Rationalize differences based on standard organic chemistry principles.



2. Two possible structures of cyclobutadiene are shown below. Apply Huckel analysis to both structures to derive the energy diagram. For **3** assume that H_{ij} for carbons connected by the double bond is β , and the carbons connected by a single bond is $\beta/2$. According to the diagrams which structure is more stable?



2



3

3. Consider the σ -framework for BH_3 and the empty p_z orbital on B. Using Huckel theory, construct a MO diagram for BH_3 .
4. Review the selection rules for allowed cycloadditions (Cotton 188-201). Do problem 7.6, pg 203 in Cotton.
5. Determine the possible hybrid orbitals of Fe in $Fe(CO)_5$, and construct the orthonormal set of hybrid σ orbitals from the atomic orbitals of Fe.