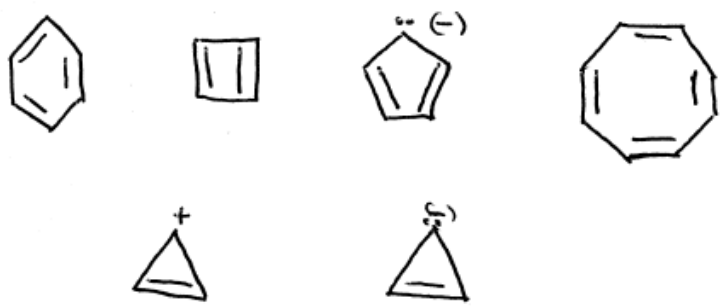
CHEM 550
Homework 10. Due Thursday. Dec. 10 at 5pm in Prof. Ginger's mailbox.
A soft one to let you rest up for the final. If you want to save yourself time on the final I recommend making sure you have complete solutions to the previous Maple exercises presented throughout the term.

CIRCLE YOUR ANSWERS AND KEY INTERMEDIATE RESULTS
STAPLE YOUR PAPERS TOGETHER
INCLUDE ALL COMPUTER PRINTOUTS

1) Use Hückel MO theory to estimate if the linear state (H-H-H+) or triangular state (each H bonded to two others in a triangle) of H_3^+ is more stable. Repeat for neutral H_3 and for H_3^-

2) Verify the equivalence of secular determinants and the geometric 'Frost Circle' method (which is a geometric realization of the general form of the 'circulant' type secular determinants that result). *Explicitly* calculate the MO Energy levels (and draw the labeled MO energy levels) for the cyclopentadienyl radical ($C_5H_5^{\cdot}$), and benzene BOTH by writing down and solving their secular determinants in the Hückel approximation, and by using the 'Frost Circle' method.

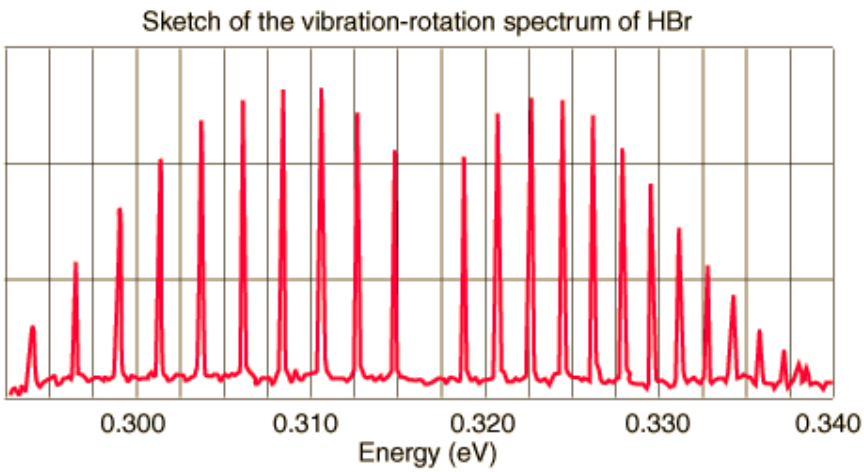
3) Draw MO diagrams, fill with e- according to Hund's rule, and deduce which of the following molecules are aromatic, radicals, or diradicals (use Hückel's 4n+2 rule):



4) In our derivation of Bloch's Theorem we will define the 'displacement' operator, *D,* as having the effect: *D*f(x)=f(x+a), and it will be associated with a potential of the form *V(x)=V(x+a)*. Prove that [D,H]=0, and *thus that simultaneous eigenfunctions exist for D and H.*

4) a) Explain in relation to the Einstein emission and absorption coefficients, why a laser requires a population inversion to sustain laser action.
b) Explain why it is very difficult to make a conventional two-state laser for short wavelength light. Calculate the ratio of the Einstein coefficients for stimulated emission and absorption for 70.8 pm x-rays, and 500 nm visible light.

5) Explain the general shapes of the following spectra, and label the peaks in each transition with the initial and final rotational/vibrational/electronic quantum #'s as appropriate.
a) infrared:



b) visible: