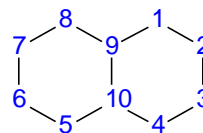


ASSIGNMENT 5

DUE: March 7, 2000



1. For naphthalene (numbering scheme shown above), set up the Hückel matrix, using $\mathbf{b} = 1$ and $x = (\mathbf{a} - \mathbf{I}) / \mathbf{b}$.
2. Using Maple (or something else) obtain the eigenvalues and eigenvectors of the Hückel matrix. Use the matrix from question 1, and set $x=0$, since all the eigenvalues are usually relative to \mathbf{a} in Hückel theory. With some fiddling, (exporting the output as a text file, editing the text file) you should be able to get the numbers into a spreadsheet for further calculations.
3. Calculate the total π electron energy, and compare it to the energy of five isolated double bonds.
4. There are four unique types of bond in naphthalene - calculate the bond order for each of them.
5. For the radical anion, estimate the unpaired electron density at the three different types of carbon. Remember that the π electron charge is given by the following equation.

$$\text{charge on atom } i = \sum_k^{\text{occupied } MOs} n_k c_{ik}^2$$