Chem 302 Laboratory 5

Numerically Solving The Schrodinger Equation for

Simple Molecular Orbitals: The Huckel Model

NAME:

In molecular quantum mechanics we want to solve the Schrodinger equation (or some variant of it) in matrix form

**HC** = **CE**

"Solving" the above equation means determining the MO coefficient matrix **C** and MO energy matrix **E**. **C** is the "eigenvector matrix" and **E** is the (diagonal) "eigenvalue matrix". **H** is the "Hamiltonian matrix" composed of elements



The Hamiltonian matrix is symmetric so *Hi,j* = *Hj,i*. Eigenvectors are orthonormal in quantum mechanics, which in matrix form means **C**T**C** = **CC**T = **I**, the identity matrix (a matrix with 1s on the diagonal and 0s every where else). The "transpose" of **C** is its inverse, **C**T= **C**-1. Considering the "orthonormality" of **C** we can then write

**C**T**HC** = **E**

We say **C** diagonalizes **H**. The process of determining **C** and **E** is "diagonalization".

Write down the Huckel Hamiltonian matrix for the following molecular skeletons (easiest to copy and paste from Excel):

Enter each of these matrices into R and obtain its eigenvalues (**E**) and eigenvectors (**C**). Copy and paste them here.

For each eigenvector matrix you obtained compute **C**T**C** and **CC**T. (HINT: Remember in R matrix multiplication is performed with the %\*% operator, and transposition is the t() function). Do the results make sense? Why?

Use R to evaluate **C**T**HC** for each molecule. Do you get **E**? Copy and paste the result here.

For each molecule, sketch the MOs, MO energy diagram (include the electrons) and speculate at to whether or not the molecule could be made in the lab. Explain your reasoning.