Chem 302 Laboratory 5

Numerically Solving The Schrodinger Equation for

Simple Molecular Orbitals: The Huckel Model

NAME:

1. For each molecular skeleton, choose the corresponding Huckel Hamiltonian matrix.
2. Enter the Huckel matrix for each molecule into R and obtain its eigenvalues (**E**) and eigenvectors (**C**).
3. 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.