Chem 302 Laboratory 5

Numerically Solving The Schrodinger Equation for

Simple Molecular Orbitals: The Huckel Model

NAME:

1. For each molecular skeleton, write the corresponding Huckel Hamiltonian matrix.

Chart, line chart

Description automatically generated

1. Enter the Huckel matrix for each molecule into R and obtain its eigenvalues (**E**).
2. For each molecule sketch the MOs
3. For each molecule sketch the MO energy diagram (include the electrons)
4. For each molecule compute the total Huckel energy.
5. For each molecule speculate whether or not the molecule could be made in the lab.