

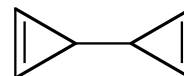
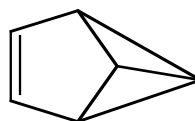
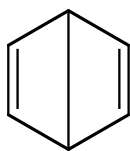
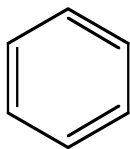
Computers in Chemistry-CHEM 3111

October 25, 2002: Lab exercise in using Spartan & ChemDraw: Geometry optimization and Semi-empirical methods.

For this exercise, you will need to locate the handful of computers in the Computer Lab that have PCSpartan installed.

You should turn in a "MSWord" document containing the data and graphics you generate.

1. Open a "Builder Window" and practice making various molecules. Use the "Minimize Energy" option to optimize the geometry using the MM2 force-field.
2. Build the following "Dewar" structures: Using the MM2 force-field, Minimize the energy of each.
 - a. What is the "Strain Energy" of each molecule (this is the result of MM2 Calculation)
 - b. Save Each molecule. Now, set up AM1 calculations for each molecule and report the heat of formation at the geometries you calculated.



3. The following "Molecular Rectifier" molecule was synthesized by Tour's group at Rice. They demonstrated that by placing the molecule between two gold leads, they could make a molecular switch or simple logic gates. Using Spartan, perform AM1 calculations on this molecule, optimizing its geometry. Then, under the "Surfaces" option, generate the "HOMO" and "LUMO" molecular orbitals. Be somewhat artistic, and make some nice orbital plots. Can you predict what happens to this molecule when it is in its first excited state? What sort of geometric arrangement do you expect?

