Molecular Electronic Structure: G94W

Purpose

The purpose of this experiment is to become somewhat familiar with perhaps the most famous *ab initio* electronic structure program available and to learn a little about the usefulness of molecular electronic structure calculations.

Equipment and Chemicals

A PC running G94W and a printer.

Directions

See the instructor for a detailed description of output from G94W.

Calculations

Run file **2_01** which is the input file for a single point energy calculation on Propene. Determine the following information from the output:

- What is the standard orientation of the molecule? In what plane do most of the atoms lie?
- What is the predicted Hartree-Fock energy?
- What is the magnitude and direction of the dipole moment for propene?
- Describe the general nature of the predicted charge distribution.