

Molecular Potential Energy Curves

Purpose:

The purpose of this experiment is to become more familiar with the *ab initio* electronic structure program G94W and molecular electronic potential energy curves.

Equipment and Chemicals:

A PC running G94W and a printer.

Directions:

See the instructor for a description of input for G94W.

Calculations:

Run file **8_02aa** which is the input file for a scan of the potential energy surface of HC. Perform the following:

- Plot the Energy [E (UHF)] from the output file versus 'R' the bond length of HC.
- Estimate (graphically) the bond dissociation energy of HC.