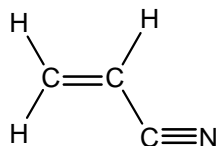


## Small Molecule Vibrational Spectroscopy

**Concept.** You will build, optimize, and carry out a force constant vibrational calculation on acrylonitrile ( $\text{H}_2\text{C}=\text{CHCN}$ ). You will be able to compare the computed results to the experimental numbers/spectra for this molecule.

**Procedure.** Build and optimize acrylonitrile using both AM1 and RHF/6-31G\*. Visualize and identify the various vibrational modes. In your results description, record frequencies and atomic motions of the vibrational modes at each level of theory, and compare to experimental numbers.



**Literature.** Compare the computed vibrational bands to those found in the literature.