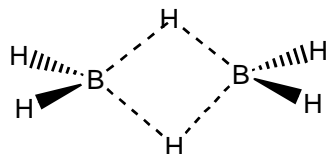


Small Molecule Vibrational Spectroscopy

Concept. You will build, optimize, and carry out a force constant vibrational calculation on diborane (B_2H_6). You will be able to compare the computed results to the experimental numbers/spectra for this molecule.

Procedure. Build and optimize diborane 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.