5.1: Overview

Learning Objectives

- Students will learn to use Orca and Avogadro to calculate and visualize the vibrational modes in the IR spectrum of simple organic molecules.
- Students will be able to describe the molecular motion involved in IR absorbances.

Overview: This exercise seeks to help you visualize what is occurring with the IR spectra of organic compounds at the molecular level. IR spectra arise from molecular vibrations that are characteristic of each compound. This is particularly useful for organic chemists seeking to determine the structure of a molecule. In this exercise you will model the vibrational spectrum of a molecule and visualize the vibrations giving rise to specific resonances. To accomplish this, we will use the quantum chemistry package called Orca to calculate the vibrational modes of hexane.[1–3] This predicted spectrum will be visualized in Avogadro and compared to the experimental IR spectrum of hexane to help assign its vibrational modes.[4,5]

Faculty Notes: This exercise is designed to help students better understand the molecular vibrations that underlie IR spectroscopy. Before completing this exercise, students should have been introduced to the concept of IR spectroscopy and basic interpretation using spectral tables. A standard desktop computer takes about 5 minutes to run the computation in this exercise. Overall, the exercise should take students about an hour to complete.