1.1: Overview

Learning Objectives

- After completing this exercise students will be able to draw simple molecules and optimize their geometry in the Avogadro molecule editor.
- Students will be able to predict the geometry of a carbon atom (or heteroatom) using VSEPR theory and compare the bond angles to a molecule simulated in the Avogadro molecule editor.

This exercise seeks to help you reinforce the concept of molecular and electronic geometry and visualize molecules in 3-dimensions. To do this we will be introducing the use of Avogadro, an open-source program designed to edit and draw molecules in 3-dimensions.[1,2] This program will allow us to estimate geometries and measure bond lengths and bond angles. We will then compare these bond angles and molecular geometries to those predicted using valance shell electron pair repulsion theory (VSEPR).

Faculty Notes: This exercise is designed to help students visualize molecules in three dimensions and cement the concepts of VSEPR theory. This exercise is designed to be completed when students are learning about the molecular and electronic geometry of simple organic molecules. Because this work is primarily concerned with VSEPR in in the context of introductory organic chemistry, 5 coordinate and greater geometries will not be covered. This exercise takes students about 30 minutes to complete.