

6.1: Overview

Learning Objectives

- Students will rotate molecules using Avogadro to aid in their understanding of how chiral centers exist in three-dimensional space.
- Students will examine the energy difference between enantiomers and diastereomers to cement the concept of differing properties of stereoisomers.

Overview: This exercise seeks to help you develop spatial skills that you will need to understand the three-dimensional structure of molecules. This is particularly important for visualizing and assigning chiral centers, where rotating the lowest priority back into the plane of the page is a vital, and often challenging, part of determining absolute configuration. Using Avogadro we can demonstrate how rotation effects chiral centers, making it easier to repeat this process in your mind's eye.^{1,2} Moreover, we will use energy calculations, performed in Orca, to examine energy differences between sets of enantiomers and diastereomers.³⁻⁶

Faculty Notes: This exercise is designed to help students with the skills needed to rotate and view molecules from different perspective in three dimensions. Additionally, this exercise seeks to highlight the energetic differences between a set of enantiomers and a set of diastereomers. Before completing this exercise, students should have been introduced to the concept of chirality and chiral centers as well as the process of assigning the absolute configuration of chiral centers. Moreover, students should have learned to determine the relationship between two stereoisomers. This exercise should take students about an hour to complete.

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