4.1: Overview

Learning Objectives

- Students will be able to use Avogadro to visualize 1,3-diaxial steric interactions by using space filling molecular models.[4,5]
- Students will use Orca to calculate the energy of substituted cyclohexane conformers.
- Students will learn to convert the ΔG° of an equilibrium into an equilibrium constant.

Overview: This exercise will help you to understand the underlying energetics behind the conformations of substituted cyclohexane chair conformations. In the lecture portion of this course, you learned that cyclohexane rings exist as an equilibrium between chair conformers that put substituents in axial or equatorial positions. Moreover, you learned that the cyclohexane chair equilibrium favors the conformer that places the bulky substituent in the equatorial position because it avoids a type of steric strain known as a 1,3-diaxial interaction. In this exercise, you will calculate the energy of both axial and equatorial cyclohexane chair molecules and convert that information into the "A" value for that substituent. You will then determine the equilibrium constant between axial and equatorial conformers of a substituted cyclohexane. To do this we will use the quantum chemistry package Orca to measure the energy of cyclohexane conformers using Density Functional Theory.[1–3]

Faculty Notes: This exercise is designed to help students understand how stability in organic chemistry relates to an equilibrium constant. Specifically, students will learn how differences in energy relate to equilibrium position. Moreover, students will use Avogadro to help visualize the steric interactions causing the 1,3-diaxial interactions. Before completing this exercise, students should have learned to draw both conformers of a substituted cyclohexane ring. A standard desktop computer takes about 50 minutes to calculate the geometry and energy of a cyclohexane chair conformer. Computational time can be decreased by encouraging students to run both calculations simultaneously. Moreover, if students are working in groups, they can distribute the calculations over more than one computer. Overall, this exercise should take students from 1.5 to 2 hours to complete.