8.1: Overview

Learning Objectives

- Students will be able to use implicit solvation in Orca to add energy of solvation to their energy calculations.[1–3]
- Students will be able to describe energetically why E2 and SN2 reactions proceed more quickly in polar aprotic solvents than in polar protic solvents.

Overview: This exercise seeks to help you understand the role that solvent can play in the energetics of a reaction. SN2 and E2 reactions are favored by conditions such as high concentrations of reactants and polar aprotic solvents. On the other hand, SN2 and E2 reactions are disfavored by polar aprotic solvents. This disparity is the result of nucleophiles (or bases) being stabilized through strong intermolecular forces with polar protic solvents. In this exercise we will calculate the energies involved in the E2 reaction of 2-chloro-2-methylpropane with a hydroxide ion. We will contrast these energies as measured in water, a polar protic solvent, and dimethylsulfoxide (DMSO), a polar aprotic solvent. This data will illustrate why polar aprotic solvents accelerate SN2 or E2 reactions.

Faculty Notes: This exercise is designed to help students understand the effects of solvation on substitution and elimination reactions. Before assigning this exercise, students should have learned about the mechanism of both bimolecular and unimolecular substitution and elimination reactions. Specifically, students should be able to predict the predominant reaction mechanism given a set of conditions. A standard desktop computer takes about 30 seconds to calculate the solvation energy for each set of conditions. Overall, the exercise should take students about 1.5 hours to complete.