11.1: Overview

> **◑ Learning Objectives**
>
> - Students will be able to draw a direct comparison between the selectivity of a reaction and the free energy of activation ($\Delta G^{\ddagger}$) of the rate determining step of the reaction.
> - Students will be able to indicate which directing groups have the greatest impact upon selectivity and how this selectivity correlates to reaction rate.

Overview: This exercise seeks to help you understand the root of selectivity in electrophilic aromatic substitution. Specifically, you will analyze data for the rate determining breaking of aromaticity in the electrophilic aromatic nitration of toluene and 1-methoxy-2-methyl-3-nitrobenzene. From these analyses you will compare the stability of the resonance stabilized σ (sigma) complexes and how they relate to the transition states separating them from the starting arene.

Faculty Notes: This exercise is designed to help students better understand the underlying cause of ortho/para or meta selectivity in an electrophilic aromatic substitution reaction. Before assigning the exercise, students should have covered the concept of electron-donating and electron-withdrawing arene substituents and their effect of rate of reaction and selectivity. This exercise should take students about an hour to complete.