

12.1: Overview

Learning Objectives

- Students will be able to use Orca¹⁻³ to calculate the energy of starting materials and products of nucleophilic opening of cyclic ethers.
- Students will determine if the extent of angle strain in a cyclic ether influences the rate at which a nucleophile can open the ring.
- Students will build intuition relating the amount of ring strain in a molecule to its reactivity.

Overview: This exercise seeks to help you understand the role that the release of strain plays in the reactivity of epoxides. Specifically, HO- or RO- are typically poor leaving groups when engaged in substitution reactions. One exception is the epoxide also known as an oxirane whose ring strain allows RO- to act as an effective leaving group. In this exercise, you will calculate the activation energy of a nucleophile opening 3-membered and 4-membered cyclic ethers.

Faculty Notes: This exercise is designed to help students better understand how ring strain influences electrophilicity of ethers. Before assigning this exercise, students should have learned SN2 reactions as they apply to epoxide opening. Please note that in the interest of computation time, this exercise is run at a relatively low-level of theory (semi-empirical). While the reaction energies show the trend needed to illustrate the core concept of the exercise, the values of ΔG° and ΔG^\ddagger should be viewed with the level of theory in mind. On a standard desktop computer, the calculation in this exercise takes about 20 minutes. Overall, this assignment should take students about an hour to complete.

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