

10.1: Overview

Learning Objectives

- Students will be able to use Orca¹⁻⁴ and Avodagro^{5,6} to calculate and visualize the molecular orbitals of cinnamic acid.
- Students will be able to relate the HOMO-LUMO gap of a compound to the wavelength of light necessary to cause the promotion of an electron,

Overview: This exercise seeks to help you understand how the frontier molecular orbitals interact to allow for a light-mediated [2+2] cycloaddition. Specifically, you will calculate and examine the molecular orbitals of cinnamic acid to determine which orbitals will overlap to form the [2+2] cyclized product, truxillic acid. From these data you will calculate the wavelength of light required to mediate the [2+2] cycloaddition between two molecules of cinnamic acid to yield truxillic acid.

Faculty Notes: This exercise is designed to help students better understand the molecular orbital overlap required for a successful 2+2 cycloaddition. Before assigning this exercise, students should have learned the basic concepts of Frontier Molecular Orbital Theory, and the mechanism of [2+2] and [4+2] cycloaddition reactions. Using a standard desktop computer, the computation in this exercise takes 45 minutes. Overall, this exercise should take students about an hour and 15 minutes.

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