3.1: Overview

Learning Objectives

- Students will be able to use Orca and Avogadro to generate molecular orbital diagrams of simple molecules containing common functional groups.
- Students will be able to identify HOMO's and LUMO's (Frontier Molecular Orbitals) of molecules and relate these to where reactions are likely to occur.
- Students will be able to relate their simplified molecular orbital diagrams of portions of molecules to those generated *in silico* (on a computer).

Overview: This exercise will help you to better understand the concept of molecular orbital theory and visualize bonding and antibonding molecular orbitals. In the lecture portion of organic chemistry, you will have learned how to predict the geometry of molecular orbitals for specific functional groups (*e.g.* carbonyls, C-Br bonds etc.). While this approach is extremely useful for determining the general shape of these orbitals, it isn't always convenient for molecules with large numbers of atoms. Moreover, this approach doesn't allow for the calculation of energy levels of molecular orbitals. The power of modern computers allows us to calculate the molecular orbitals of a small molecule in a few minutes. To do this, we will be using the quantum chemistry package called Orca to calculate the molecular orbital shapes and energy levels.[1–3] After this calculation, we will visualize the orbitals and read their energies using Avogadro. [4,5]

Faculty Notes: This exercise is designed to help students understand the shapes and energy levels of molecular orbitals. Specifically, this is designed to complement an introductory discussion of molecular orbital theory where students are taught to generate simplified molecular orbitals for diatomic molecules and/or two atom functionality of a more complex molecule. Before completing this exercise, students should have been exposed to the basics of molecular orbital theory including the HOMO and LUMO terminology. A standard desktop computer takes about 30 seconds to run the computation in this exercise. Overall, the exercise should take students about an hour to complete.