

2.1: Overview

Learning Objectives

- Students will be able to predict which bonds on a line bond structure will have partial double bond character.
- Students will be able to use Avogadro and Orca to calculate and visualize the geometry of molecules using density functional theory.

Overview: This exercise seeks to reinforce the idea of resonance in describing the electronic structure of simple organic molecules. To do this, we will model simple molecules which do and do not have significant resonance using the Orca and Avogadro software packages.¹⁻⁵ This exercise shows that molecules with significant resonance structures often have what is referred to as partial double bond character.

Faculty Notes: This exercise is designed to help students grasp the concept of resonance structures and resonance hybrids in the description of molecules with delocalized electrons. It is recommended that the concept of resonance structures and the arrow pushing required to interconvert them be covered in lecture prior to assigning this activity. A standard desktop computer takes about 6 minutes to run the computation in this exercise. Overall, the exercise should take students about an hour to complete.

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