

# TABLE OF CONTENTS

## Licensing

### 1: Introduction to Avogadro

- 1.1: Overview
- 1.2: Background
- 1.3: Computational Instructions
- 1.4: Exercise Questions

### 2: Bond Lengths and Resonance

- 2.1: Overview
- 2.2: Background
- 2.3: Computational Instructions
- 2.4: Exercise Questions

### 3: Visualizing Molecular Orbitals with Avogadro and Orca

- 3.1: Overview
- 3.2: Background
- 3.3: Computational Instructions
- 3.4: Exercise Questions

### 4: Measuring Equilibrium on Cyclohexane Chair Structures

- 4.1: Overview
- 4.2: Background
- 4.3: Computational Instructions
- 4.4: Exercise Questions

### 5: Computing and Visualizing Infrared Spectra of Organic Molecules

- 5.1: Overview
- 5.2: Background
- 5.3: Computational Instructions
- 5.4: Exercise Questions

### 6: Manipulating of Molecules in Three Dimensions

- 6.1: Overview
- 6.2: Background
- 6.3: Computational Instructions
- 6.4: Exercise Questions

### 7: Thermodynamics, Kinetics, and the Reaction Coordinate Diagram

- 7.1: Overview
- 7.2: Background
- 7.3: Computational Instructions
- 7.4: Exercise Questions

## 8: Understanding the Effect of Solvation on E2 Reactions

- 8.1: Overview
- 8.2: Background
- 8.3: Computational Instructions
- 8.4: Exercise Questions

## 9: Calculating Bond Dissociation Enthalpy and Analyzing the Radical Chlorination of Norbornane

- 9.1: Overview
- 9.2: Background
- 9.3: Computational Instructions
- 9.4: Exercise Questions

## 10: Examining the Synthesis of Naturally Occurring Cyclobutane Compounds

- 10.1: Overview
- 10.2: Background
- 10.3: Computational Instructions
- 10.4: Exercise Questions

## 11: Examining the Energetics of Selectivity in Electrophilic Aromatic Substitution

- 11.1: Overview
- 11.2: Background
- 11.3: Computation Assignment and Exercise Questions

## 12: Measuring the influence of ring strain in ether substitution

- 12.1: Overview
- 12.2: Background
- 12.3: Computational Instructions
- 12.4: Exercise Questions

[Index](#)

[Glossary](#)

[Detailed Licensing](#)