

# Chemistry 6300    Advanced Modern Organic Chemistry    Fall Semester 2021

**Instructor:** Dr. Alvan C. Hengge, 343 Widtsoe, 7-3442, [alvan.hengge@usu.edu](mailto:alvan.hengge@usu.edu)

**Schedule:** MWTh, 11:30 am - 12:20 pm, in Widtsoe 330

**Course Content and Objectives:** The course focuses on understanding chemical reaction mechanisms, and learning the methods used to discover the mechanisms by which chemical reactions occur.

**No Textbook** is required; required reading materials will be posted on Canvas in pdf format. Some will be literature papers; others will be individual chapters from physical organic chemistry textbooks. Two books we will use chapters from are:

Perspectives on Structure and Mechanism in Organic Chemistry, Second Edition, by Felix Carroll

Modern Physical Organic Chemistry, by Anslyn and Dougherty

**Exams:** There will be two exams during the semester and a final exam; each exam will count equally. There will be problem sets assigned for homework approximately weekly; solutions will be discussed in class with students sent to the whiteboard to show their solutions. Collaboration on the homework problems is encouraged. These will not be turned in for grading, but, active participation during group discussion of these problem sets is required and will be factored into assigning final grades. The course grade will be based on the exams and participation during problem solving sessions.

**Withdrawal Policy:** The same as the USU policy.

**Missed Exams:** There are no make-up exams. If one exam is missed, the grade will be determined from the other two exams. Students must take two of the three exams, one of which must be the final, to receive a passing grade.

**A comprehensive final exam will be scheduled early in the week of December 13.**

## Learning Objectives

During this course, you will learn:

- Correct practices for electron pushing and mechanism writing, and how to recognize viable intermediates in reactions.
- The characteristics, formation, and chemical behavior of carbocations, carbanions, radicals and carbenes, including migrations, rearrangements, and neighboring group participation.
- Fundamental principles that control rates and mechanisms of chemical reactions
- How to distinguish a likely mechanism from an unlikely one; to distinguish chemically reasonable intermediates from unreasonable ones; how to write sound arrow-pushing mechanisms with correct electron accounting.
- How to design experiments to gain mechanistic information about reactions, and how to interpret the results.
- How to construct and interpret reaction coordinate diagrams, and More-O'Ferrall-Jencks diagrams, to represent chemical reaction mechanisms.
- How to derive, test, and interpret basic rate laws for chemical reactions.
- How to design experiments to obtain activation parameters (enthalpy and entropy of activation) for reactions; linear free energy relationships and kinetic isotope effects; how to interpret such data to draw mechanistic conclusions.
- The application of basic molecular orbital theory; the use of frontier molecular orbitals and the Woodward-Hoffman rules to explain and predict the outcome of electrocyclic reactions, cycloaddition and cycloreversion reactions, and sigmatropic reactions.

Course Outline: the table below gives course topics and the associated required readings. Chapters from the Anslyn & Dougherty text are designated by the abbreviation “A & D.” chapters from the Carroll text are designated as “Carroll.” All required reading materials are posted on Canvas, together with supplemental reading materials for students who want to dive deeper into particular subjects.

### Lecture Topics

Mechanism Writing and Electron Pushing

Reactive Intermediates; Reactions and Rearrangements of:

radicals  
carbenes  
carbocations  
carbanions

----- exam 1 -----

Methods of Studying Reaction Mechanisms

General methods for determining reaction mechanisms  
Kinetics and rate laws  
Thermodynamics  
Measurement & interpretation of activation parameters  
Reaction barriers and potential energy surfaces  
Isotope effects  
Linear free energy relationships: Hammett, Brønsted/Leffler

----- exam 2 -----

Pericyclic Reactions

electrocyclic reactions  
sigmatropic reactions  
cycloaddition and cycloreversion reactions  
other electrocyclic reactions

### Required Reading

Appendix 5 A & D.

Carroll Chapter 5.2  
Carroll Chapter 5.3  
Carroll Chapter 5.4  
Carroll Chapter 5.5

A & D Chapter 8.8

Carroll Chapter 6 : sections 6.1 – 6.6,  
and 6.8

A & D Chapter 7: sections 7.1, 7.2,  
7.4, 7.5, and 7.8.2

A & D Chapter 8: sections 8.1, 8.3,  
8.5

Pericyclic Reactions

Sigmatropic Rearrangements

**Student Disability Policy:** Students with physical, sensory, emotional or medical impairments may be eligible for reasonable accommodations in accordance with the Americans with Disabilities Act and Section 504 of the Rehabilitation Act of 1973. All accommodations are coordinated through the Disability Resource Center (DRC) in Room 101 of the University Inn, 797-2444 voice, 797-0740 TTY, or toll free at 1-800-259-2966. Please contact the DRC as early in the semester as possible. Alternate format materials (Braille, large print or digital) are available with advance notice.