



UNIVERSITY OF  
CALGARY

UNIVERSITY OF CALGARY  
FACULTY OF SCIENCE  
DEPARTMENT OF CHEMISTRY  
FALL 2018

- 1. Course:** CHEM 659.28, Selected Topics in Organic Chemistry (Molecular Structure and Reactivity)  
Lecture Section: L02  
T/Th, 11-12:15, ST 125, Dr. Van Humbeck (SB 229A, 403.220.3039, jeffrey.vanhumbec1@ucalgary.ca)  
Office hours: By appointment

Chemistry Department Office: Science A 229, 403.220.5341, chem.info@ucalgary.ca

It is recommended that students use their U of C account for all correspondences.

D2L: CHEM 659.28 L02-(Fall 2018)-Selected Topics in Organic Chemistry

- 2. Course Description**

This course is designed with a single goal in mind: to provide graduate students with a full suite of tools that will allow them to study the mechanism of any reaction they encounter in their research work. To achieve this goal three specific skills will be delivered, which reflect the division of the course into three units. The dates of midterm exams will not change, but all other dates are subject to change.

*(i) Theoretical Groundwork for Mechanistic Experiments (Unit 1 Exam: October 4, 2018)*

To understand which experimental tools can be properly applied in any particular context, the theoretical underpinnings of the experiments themselves must be discussed. Over the course of seven lectures, the following topics will be presented:

September 6: Introduction and Reaction Coordinate Diagrams  
September 11/13: Transition State Theory and the Hammond Postulate  
September 18/20: Rate Laws  
September 25/27: Electron Transfer Theory and Processes

*(ii) Experimental Techniques for Mechanistic Study (Unit 2 Exam: November 8, 2018)*

Experimental tools both for the direct elucidation of mechanism, as well as for the efficient planning and analysis of large experimental trials will be presented. Over the course of eight lectures, the following topics will be presented:

October 2/9/11: Kinetic and Thermodynamic Isotope Effects, Labelling, and Crossover  
October 16/18: Linear Free Energy Relationships  
October 23: Design-of-Experiments (DOE) Strategies for Chemistry  
October 25: Introduction to Basic Principles of Machine Learning  
October 30: Applications of Machine Learning in Chemistry

*(iii) Orbital Effects and Reactive Intermediates*

The confirmation or rejection of any particular mechanism relies upon a **prediction** not matching experimental results. So, the ability to predict how basic changes in molecular structure will affect the corresponding molecular orbitals—and, therefore, molecular reactivity—is crucial. The concept of organic group orbitals and qualitative molecular orbital theory (QMOT) will be presented over the course of seven lectures.

November 1/6: Qualitative MO Theory (QMOT)

November 20: Hyperconjugation

November 22: Cations

November 27: Anions/Radicals

November 29: Radicals/Carbenes

December 6: Photochemistry

***ALL OTHER CRITICAL COURSE INFORMATION CAN BE FOUND ON THE OFFICIAL COURSE INFORMATION SHEET***

Department Approval: Approved by Department Head Date: August 30, 2018