

**UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
FALL 2018**

1. Course: CHEMISTRY 453, Advanced Organic Chemistry

LEC	DAYS	TIME	ROOM	PROFESSOR	OFFICE	EMAIL	OFFICE HOURS
L01	MWF	11:00-11:50	ENE239	T.G. Back	SB 217	tgback@ucalgary.ca	TBA

To avoid IT problems, it is recommended that the students use their U of C account for all course correspondence.

Departmental Office: Room SA 229, Tel: (403) 220-5341, e-mail: uginfo@chem.ucalgary.ca

- 2. Course Description: Lectures:** Hückel MO theory. Molecular mechanics principles. Frontier MO interactions and their application to: electrocyclic reactions, cycloadditions, sigmatropic rearrangements. Woodward-Hoffmann rules for pericyclic reactions. Photochemistry. Reactive intermediates (carbocations, free radicals, carbanions, carbenes and nitrenes, as time permits). Methods for studying reaction mechanisms.

Laboratory: Synthesis, photochemistry, molecular modeling

- 3. Recommended Textbook:** "Advanced Organic Chemistry" by B. Miller, Pearson-Prentice Hall, 2nd edition (2004). (available from Bound & Copied)

4. Topics Covered and Suggested Readings:

The first entry below (Jones) is the textbook used in recent years for Chemistry 355 and it will be useful for looking up background material; the other texts are also available from the Bookstore. The second entry (Miller) is the recommended text for Chem 453. It provides coverage of course material except for Huckel MO Theory and Molecular Mechanics. The third entry (Hehre) is optional and provides useful further information about computational methods such as those used in the Molecular Modeling experiments.

1. "**Organic Chemistry**" by M. Jones, 3rd ed., Norton, New York (2005) or later editions, or any similar textbook.
2. "**Advanced Organic Chemistry - Reactions and Mechanisms**" by B. Miller, Prentice-Hall 2nd edition (2004).
3. "**The Molecular Modeling Workbook for Organic Chemistry**" by W.J. Hehre et. al., Wavefunction, Inc. (1998).

The following texts contain supplementary material that is relevant to the course. Students are advised to consult them for additional information and insight into the material presented in lectures. They are available in the Reserve Reading Room of the library as well as in the Bookstore.

4. "**Mechanism and Theory in Organic Chemistry**" by T.H. Lowry and K.S. Richardson, Harper & Row, N.Y. (1976), or later editions.
 5. "**Orbital Interaction Theory of Organic Chemistry**" by A. Rauk, J. Wiley & Sons, N.Y. (1994).
 6. "**Frontier Orbitals and Organic Chemical Reactions**" by I. Fleming, J. Wiley & Sons, Chichester (1976).
- 4. Laboratory Experiments:** (12 weeks, 4 hours/ week) Modeling organic structures and reactions using molecular mechanics and MO methods. Synthetic projects designed to illustrate basic principles: Synthesis of Azulene. Photochemical Synthesis of Benzopinacol. Chemiluminescence. Research project combining both experimental and theoretical approaches: Resolution of Racemic Ibuprofen.

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