Course Syllabus

Edit

CHM 348H: Organic Reaction Mechanisms: Fall 2020

Classes: Tuesdays and Thursdays 2-3 p.m., room Lash Miller (LM) 158: in-person section. Virtual session at same time. Tests will be required during class time.

COURSE OVERVIEW: CHM 348H provides concepts and methods that allow us to understand how and why chemical reactions occur, based on the principles of well-established theories and analyses. The course also introduces modern concepts of structure and stereochemistry. The virtual laboratory provides an opportunity to apply the concepts of the course in a practical setting. It is a central aspect of the course, providing insights and experience in the topics covered in the classes and readings. The virtual laboratory focus is on the mechanistic interpretation of experimental and computational measurements, and clear communication of findings through the construction of formal reports.

Classes will cover these general areas: advanced stereochemical principles, molecular mechanics, molecular orbitals and their diverse applications (including pericyclic reactions, aromaticity, and photochemistry), kinetics and mechanisms, transition state theory, catalysis by acids and bases, quantitative substituent effects, and examples of the basis of reaction mechanisms for diverse types of compounds. The nature of reactive intermediates as implied by theory and experiment will be a focus throughout the course. The approach taken is not limited to organic chemistry and the ideas can be applied to structure and mechanism in any area of chemistry.

Information is made available through the classes, reading from the texts, reading from additional material, and assigned problems. Slides used in classes are available to reduce copious note-taking, but they do not provide a substitute for reading the texts and doing problems.

LEARNING OUTCOMES: By the end of the course, students will be expected to be able to:

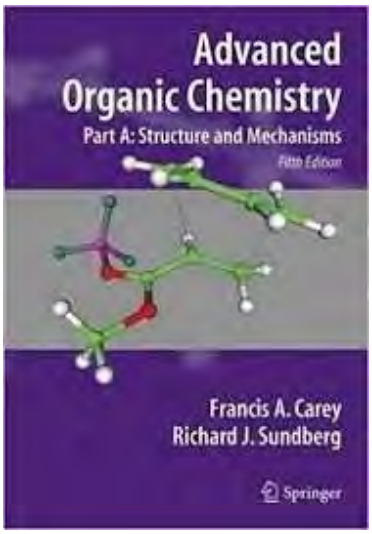
- apply modern understanding of stereochemistry, emphasizing the basis of possible and impossible distinctions, and the effects of chirality and prochirality
- utilize the concepts of molecular orbital theory and their application to the consideration of potential reaction pathways
- apply appropriate experimental and computational methods to test mechanistic hypotheses

- propose all potential mechanisms for the reaction of interest
- consider the results of experimental measurements and calculations that exclude proposals that are inconsistent with those results
- demonstrate an understanding that effectively tests the results of novel theories
- expand their knowledge of organic chemistry to include those that contain the general conceptual foundations of physical chemistry, including classical and quantum mechanical effects on reactivity
- apply rigorous and/or approximate methods to propose possible pathways and how to test each of them. Examples include intrinsic barrier theory, orbital symmetry, multidimensional energy diagrams, and no barrier theory

TEXTBOOK: Carey & Sundberg, Advanced Organic Chemistry Part A (paperback version in the U of T Textbook Store, also available at no cost as an on-line version through the U of T Libraries; see below) and McMurry, Organic Chemistry, from previous courses (8th or 9th edition).

Advanced Organic Chemistry: Part A:

(https://portal.utoronto.ca/webapps/blackboard/content/listContentEditable.jsp?
86_1&course_id=_864314_1&mode=reset#)



Title	**Advanced Organic Chemistry: Part A**
Author	Francis A. Carey and Richard J. Sundberg
ISBN	978038768346-1
Publisher	Springer
Publication Date	January 1, 2007
Binding	softcover
Type	Digital
URL	http://myaccess.library.utoronto.ca/login?url=http://link.springer.com/openurl?genre=book&isbn=978-0-387-44897-8 (http://myaccess.library.utoronto.ca/login?url=http://link.springer.com/openurl?genre=book&isbn=978-0-387-44897-8)

LABORATORY OVERVIEW: The study of organic reaction mechanisms is a highly practical subject. The **mandatory** laboratory sessions closely reflect the topics addressed during class time, and are intended to provide students with opportunities to analyze various forms of data (spectroscopic, kinetic, equilibrium and computational) in order to propose reasonable reaction mechanisms and rationalize physical phenomena. Arrangements will be different in Fall 2020 compared to previous years as, due to safety and space limitations, it will not be possible to offer in-person laboratory work. All practical sections will be on-line virtual activities: students will be graded on individual laboratory reports. The nature of the activities and their scheduling is available **here**.

ASSESSMENT: Evaluation items, including assignments (twice and final) 15%, 15%, and 30%. Laboratory attendance and reports: 30%. Class attendance and participation (whether in-person or on-line): 10%. Students are responsible for checking the time, date, and submission process for each item of term work. **A penalty of 10% of the maximum mark will be deducted daily for term work submitted past the deadline.**

RETURN OF GRADED MATERIAL: Laboratory reports, lecture tests, and other work will be graded electronically and returned to students through Quercus.

RE-GRADING: Requests for reconsideration of grading of any assignment must be submitted in writing, along with the paper, if there is one, within one week of the date in which it is returned to the class. The request must specify what any perceived errors are and how they should be corrected. Students are not permitted to submit work for re-grading if any alterations have been made to the work. and there is no process for further appeals. Please note that partial credit is given in some cases for incorrect answers. The provision and amount of any partial credit is not subject to re-grading. In the case of electronic grading, explanations will be provided.

POLICY FOR MISSED EVALUATIONS: An acceptable written petition is required, with a medical exemption form if applicable. The petition must be submitted electronically to Professor Kluger within one week of the missed evaluation. If one evaluation item of two possible items is missed with an acceptable petition, the grade on the one that is done will count for both. If both are missed, the final item will count for 60% of the overall course grade. If an evaluation item is missed without an acceptable petition, a grade of “0” will be recorded for that item. Please note that there will be no supplemental items to make up for a poor or missed performance on that item.

STUDENT HOURS: Professor Ronald Kluger: DB 444 (opposite the Chemistry Library). Normally MWF 11:30 a.m. - 12:30 p.m. Meetings via Zoom are available and are preferable. Please contact me by email (**r.kluger@utoronto.ca (mailto:r.kluger@utoronto.ca)**) in advance to confirm a meeting at those times or to request an alternative time if you have a conflict. Please do not use email for chemistry content questions: you are most welcome to arrange a virtual meeting and have a discussion instead!

Professor Andrew Dicks: available by email appointment (**andrew.dicks@utoronto.ca (mailto:andrew.dicks@utoronto.ca)**).

CLASS & ASSIGNMENT SCHEDULE: Please note that during Fall 2020, in-person classes require full compliance with all conditions imposed by the Ontario Ministry of Health, Toronto Public Health, and the University of Toronto (St. George campus) at all times. Section sizes for in-person activities have been adjusted to allow for social distancing within the assigned classroom. As a result, **only** those students registered for the in-person section should show up to the classroom.

Date	**Tuesday**	**Thursday**	**Reading (C&S = C; McMurry= M)**	**Slide Files (C&S chapter or noted)**
September 10	Classes start Thursday	Stereochemistry, molecular mechanics, conformations	C 2.1, 2.2, 2.3	Stereochemistry, Chapter 2
15, 17	Continues...	Molecular orbitals	C 1.2	Chapter 1
22, 24	Transition state theory		C 3.2	Transition state theory
29 October 1	Kinetics, reaction principles, Marcus theory, linear free energy plots, curved free energy plots		C 3.2, 3.3, 3.6	Trends and predictions CSCh3.6
October 6, 8	Isotope effects, organocatalysis		C 3.5-3.8	CSCh3 isotope effects and catalysis
13, 15	Photochemistry	**Test 1 October 15**	C 12.1	Chapter 12
20, 22	Diels Alder reactions, pericyclic processes, frontier orbitals & rules		M 14 & 30, C 10.1	McMurry Ch14 Diels Alder & Ch30 pericyclic reactions
27, 29	Nucleophilic substitution, carbocations		C 4.1, 4.3, 4.4	Chapter 4
November 3, 5	Elimination mechanisms		C 5.10	Chapter 5

November 9-13	**Reading Week (no classes)**			
17, 19	Carbanions	Carbonyl reactions	C 6.1-6.6, Decarboxylation	Chapter 6, Decarboxylation and Marcus theory
24, 26	Carbonyl reactions, assignment information	**Test 2 Nov 26**	C 7.1-7.3	Chapter 7
December 1,3	Carbonyl reactions	Catching up	C7.4-7.7	Chapter 7
Dec 7,9	Review	Catch-up if needed		

ACCESSIBILITY ACCOMMODATIONS: Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: please contact the Accessibility Services (AS) office for more information (**www.studentlife.utoronto.ca/as/services (http://www.studentlife.utoronto.ca/as/services)**). The course will provide the accommodation(s) that the AS office indicates to the instructional staff.

FINAL ASSESSMENT: The Faculty of Arts & Science has adopted a final assessment period (rather than a final examination period) during December 2020. The course final test will be scheduled during the final assessment period.

IMPORTANT COURSE POLICIES:

- Communication with instructors: please use email to arrange in-person or on-line meetings for discussions. Students must email from their U of T email account. Please allow 24 hours for a response on **weekdays.**
- All online interactions are expected to conform with the University statement regarding a positive learning environment: "*The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. U of T does not condone discrimination or harassment against any persons or communities*".
- Specific guidance regarding student technology requirements is at: **https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-**

(https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/) learning/ (https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/) . Advice for students more broadly regarding online learning is available here: https://onlinelearning.utoronto.ca/getting-ready-for-online/ (https://onlinelearning.utoronto.ca/getting-ready-for-online/) . This course requires the use of computers, and of course sometimes things can go wrong when using them. You are responsible for ensuring that you maintain regular backup copies of your files, use antivirus software (if using your own computer), and schedule enough time when completing an assignment to allow for delays due to technical difficulties. Computer viruses, crashed hard drives, broken printers, lost or corrupted files, incompatible file formats, and similar mishaps are common issues when using technology, and are not acceptable grounds for a deadline extension.

- Privacy and appropriate use of course materials: Lectures will be recorded, and the recordings made available for a limited time through Quercus. These recordings should be considered private and for the use of students registered in the course **only**. They may not be shared or re-posted in any way. Students may not make their own recordings, either for personal use or distribution. Students with accessibility requirements should contact the course instructor to make appropriate arrangements.
- Academic integrity: academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters (https://governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019 (https://governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019)) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

  In laboratory reports:

  1. Using someone else's ideas or words without appropriate acknowledgement.
  2. Submitting your own work in more than one course without the permission of the instructor.
  3. Making up sources or facts.
  4. Obtaining or providing unauthorized assistance on any assignment.

  On online written assignments:

  1. Using or possessing unauthorized aids.
  2. Looking at someone else's answers during an exam or test.
  3. Misrepresenting your identity.

  In academic work:

  1. Falsifying institutional documents or grades.
  2. Falsifying or altering any documentation required by the University.

- All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see **https://www.academicintegrity.utoronto.ca/ (https://www.academicintegrity.utoronto.ca/)**). Normally, students will be required to submit their course essays to Turnitin.com for a review of textual similarity and detection of possible plagiarism. In doing so, students will allow their essays to be included as source documents in the Turnitin.com reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of the Turnitin.com service are described on the Turnitin.com web site.