Course Syllabus

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CHM 348H: Organic Reaction Mechanisms: Fall 2021

Classes: Tuesdays and Thursdays 2:10 - 3:00 p.m. **in-person** in Lash Miller Building - room LM 158 (80 St. George Street, NE entry). There will be access to on-line synchronous sessions from 9th - 23rd September only. If you choose this option your camera **must** be on while your microphone should be muted until you ask or answer a question.:

Join Zoom Meeting (Links to an external site.)

Meeting URL: https://utoronto.zoom.us/j/83973549881 (Links to an external site.)

Meeting ID: 839 7354 9881

Laboratories: Mondays or Tuesdays 8:30 a.m. - 1 p.m., starting the week of Monday 4th October. **There is a mandatory introductory laboratory orientation session on Monday 27th & Tuesday 28th September.**

Important: tests will be administered and written in-person during class time.

Teaching Team/Contacts:

Professor Ronald Kluger (classes): r.kluger@utoronto.ca, 416-978-3582

Professor Andrew Dicks (laboratories): andrew.dicks@utoronto.ca

Student Hours:

Professor Kluger: DB 444 (opposite the Chemistry Library). Normally MWF 11:30 a.m. - 12:30 p.m. Please do not use email for chemistry content questions: you are most welcome to arrange a meeting and have a discussion instead by email request to r.kluger@utoronto.ca.

Professor Dicks is available by email request for appointment (andrew.dicks@utoronto.ca) and during all scheduled laboratory hours (MT 8:30 a.m. - 1 p.m., starting on Monday 4th October).

COURSE DESCRIPTION: CHM 348H provides concepts and methods that allow us to understand how and why chemical reactions occur using modern principles of reactions, structure and stereochemistry. A central aspect of the course, our laboratory provides insights and experience in the topics covered in the classes and readings. We focus on

mechanistic interpretation of our experimental and computational measurements, followed by clearly written interpretation through formal scientific reports.

Readings, classes and assigned problems cover important areas including: advanced stereochemical principles, molecular mechanics, molecular orbitals and their applications (including pericyclic reactions, aromaticity, and photochemistry), principles of kinetics and relations to mechanisms, transition state theory, catalysis by acids and bases, and quantitative use of substituent effects. This collection of knowledge is applied to diverse processes in specified types of compounds. The nature of reactive intermediates, as implied by theory and experiment, will be a focus throughout the course. These approaches are not limited to organic chemistry: the ideas can be applied to structure and mechanism in any area.

Required material for tests and the course final examination is presented in class and in the course textbook, as well as in additional reading from journal articles, assigned problems, laboratory preparation, experiments, and reports. Slides used in class are available to download as a framework to help with note-taking.

STUDENT LEARNING OUTCOMES: by the end of the course, successful students will be able to:

- apply modern understanding of stereochemistry, emphasizing the basis of possible and impossible distinctions, and the effects of chirality and prochirality.
- utilize 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 potential mechanisms in new areas.
- consider 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.

PREREQUISITE COURSE: CHM 348H assumes that you have a fundamental understanding of organic chemistry concepts as discussed in CHM 247H (Introductory Organic Chemistry II) or CHM 249H (Organic Chemistry). Students must have either of these credits with a minimum grade of 63%.

REQUIRED TEXTBOOKS: 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). Organic Chemistry (McMurry, used in CHM 247H/CHM 249H (8th or 9th edition)) is also required.

Advanced Organic Chemistry: Part A:

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	10.1007/978-0-387-44899-2.pdf (utoronto.ca)Links to an external site.

CLASS SCHEDULE:

NOTE: classes will be taught in-person throughout the term (although this is subject to change). Between 9th - 23rd September the in-person classes will also be accessible on-line at the same time through Zoom. More details about this will be provided prior to the first class on Thursday 9th September.

Date	Tuesday	Thursday	Reading (C&S = C; McMurry= M)	Slide Files (C&S chapter or noted)
September 9	Classes start Thursday	Stereochemistry, molecular mechanics, conformations	C 2.1, 2.2, 2.3	Stereochemistry, Chapter 2
14, 16	Continues...	Molecular orbitals	C 1.2	Chapter 1
21, 23	Transition state theory		C 3.2	Transition state theory
28 30	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 5, 7	Isotope effects, organocatalysis		C 3.5-3.8	CSCh3 isotope effects and catalysis
12, 14	Photochemistry	**Test 1 October 14**	C 12.1	Chapter 12
19, 21	Diels Alder reactions, pericyclic processes, frontier orbitals & rules		M 14 & 30, C 10.1	McMurry Ch14 Diels Alder & Ch30 pericyclic reactions
26, 28	Nucleophilic substitution, carbocations		C 4.1, 4.3, 4.4	Chapter 4
November 2, 4	Elimination mechanisms		C 5.10	Chapter 5
November 8-12	**Reading Week (no classes)**			
16, 18	Carbanions	Carbonyl reactions	C 6.1-6.6, Decarboxylation	Chapter 6, Decarboxylation and Marcus theory

23, 25	Carbonyl reactions, assignment information	**Test 2 November 25**	C 7.1-7.3	Chapter 7
29, **Dec 2**	Carbonyl reactions	Catching up	C7.4-7.7	Chapter 7
Dec 6, 8	Review	Catch-up if needed		

LABORATORY OBJECTIVES: the study of organic reaction mechanisms is a highly practical subject. The **mandatory** laboratory sessions closely reflect the topics addressed in the class part of the course. An overview of the laboratory objectives, structure and organization will be covered during the orientation sessions on 27th/28th September.

EVALUATION & GRADING SCHEME - Two (2) methods and you get the one that gives you the higher grade!

Grading Scheme 1:

- Two 50 minute ("hour") tests during class time on Thursday 14th October and Thursday 25th November where each grade counts as **15%** of the final grade.
- + Final examination (two hours) scheduled during the December final assessment period: for **30%** of final grade
- + Laboratory: attendance, observed laboratory techniques, and reports for 40% of final grade.

Grading Scheme 2:

- Two 50 minute ("hour") tests during class time on Thursday 14th October and Thursday 25th November where each grade counts as **10%** of the final grade.
- + Final examination (two hours) scheduled during the December final assessment period: for **40%** of final grade
- + Laboratory: attendance, observed laboratory techniques, and report for **40%** of final grade.
- LATENESS PENALTY for lab work:
- You are responsible for meeting the stated time, date and submission process for each piece of work. **A penalty of 10% of the maximum possible mark will be deducted daily for work submitted past due.**

RETURN OF GRADED MATERIAL & RE-GRADING REQUESTS: laboratory reports and tests will be graded and returned to students as soon as possible. Requests for reconsideration of grading for any piece of work must be submitted in writing within one week of the date in which it is returned to you. (Some incorrect answers on tests may be given partial credit - the extent of any partial credit is not subject to a request for additional credit.) The request to have an answer reconsidered or addition of points corrected must specify the correct total or why the answer has been mis-marked. Students are not permitted to submit work for re-grading if any alterations have been made to the work. There is no other appeal process within the course. In some cases, incorrect answers receive partial credit - at the discretion of the grader(s). The extent of that partial credit is not subject to reconsideration.

POLICY FOR MISSED TESTS & LABORATORY SESSIONS: T**here are no make-up term tests in CHM 348H, and there are no make-up laboratory sessions. Policies for final assessments (exams) generally allow students who petition based on a relevant medical assessment may be offered a supplemental examination or an altered grading scheme.** Students who are absent from class for any reason (e.g., COVID-19 illness, other illness or injury, family situation) and who require consideration for missed academic work should report their absence through the online absence declaration. The declaration is available on ACORN under the “Profile and Settings” menu. **A student who misses a scheduled term test must additionally contact Professor Kluger WITHIN ONE WEEK to discuss their situation.** If a student is given consideration for missing one test, the grade on the one that is written will count for both tests. If both tests are missed, the final examination will count for 60% of the overall course grade. If a test is missed without an acceptable reason, a grade of “0” will be recorded for the test. Please note that there will be no supplemental opportunities to make up for a poor or missed performance on term work. **A student who misses a scheduled laboratory session must additionally contact Professor Dicks WITHIN ONE WEEK to discuss their situation. This is a requirement to receive consideration for the missed laboratory.**

IMPORTANT COURSE POLICIES:

- each member of this course is expected to maintain a:

(i) professional and respectful attitude during all course activities, including classes, laboratories, and online activity;

(ii) personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met;

(iii) collection of notes recorded independently based on concepts covered in course activities;

(iv) familiarity with the university policy on Academic Integrity (below).

- email will generally be responded to within 24 hrs. *on weekdays*. Email will only be accepted if: (1) you send it from your utoronto.ca account; (2) you identify yourself in the email subject as a student in CHM 348H and include your name and University of Toronto student ID number; (3) no attachments are sent, unless official university correspondence is being forwarded (e.g. a letter detailing academic accommodations); (4) you are aware that organic chemistry can be talked about much more effectively through online student hours rather than by email, and that sending emails is not a substitute for attending classes.
- 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. As course instructors, we will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our Equity Offices.
- privacy and appropriate use of course materials: classes may be recorded. In the case of recorded classes, they are 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 Professor Kluger 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-1-2019Links to an external site.) 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 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/Links to an external site.). Normally, students will be required to submit their course essays to the University's plagiarism detection tool 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 tool's reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of this tool are described on the Centre for Teaching Support & Innovation web site (https://uoft.me/pdt-faq (Links to an external site.)).

ACCESSIBILITY NEEDS: students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact Accessibility ServicesLinks to an external site. as soon as possible.

ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES: following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of a test or laboratory session. Students must inform the appropriate instructor **before** the session/assignment date to arrange accommodations.

ADDITIONAL SERVICES & SUPPORT: the following are some important links to help you with academic and/or technical service and support:

- general student services and resources at Student LifeLinks to an external site.
- full library service through University of Toronto LibrariesLinks to an external site.
- resources on conducting online research through University Libraries ResearchLinks to an external site.
- resources on academic support from the Academic Success CentreLinks to an external site.
- learner support at the Writing Centre Links to an external site.
- information for Technical Support/Quercus SupportLinks to an external site.

ACKNOWLEDGEMENT OF TRADITIONAL LANDS: we wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.