# CHM 348H (Organic Reaction Mechanisms): Fall 2022 Syllabus

<u>*Classes:*</u> Tuesdays and Thursdays 2:10-3:00 p.m. **in-person only** in the <u>Galbraith BuildingLinks to an external site.</u>, 35 St. George Street: **GB 220 on Tuesdays** and **GB 120 on Thursdays**.

<u>Laboratories</u>: Mondays or Tuesdays 8:30 a.m. - 1 p.m., starting the week of Monday 3rd October. There is a mandatory introductory laboratory orientation session on the mornings of Monday 26th & Tuesday 27th September. An overview of the planned experiments is available <u>here</u>.

#### 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 <u>r.kluger@utoronto.ca</u>.

Professor Dicks is available by email request for appointments (<u>andrew.dicks@utoronto.ca</u>) and during all scheduled laboratory hours (MT 8:30 a.m. - 1 p.m., starting on Monday 3rd October).

<u>COURSE DESCRIPTION:</u> We will discuss and apply concepts and methods that allow us to understand important principles of organic chemical structure and reactivity. We will cover empirical and theoretical principles that apply generally to structure, bonding, and reaction energetics, along with illustrative examples. As the central component of the course, the laboratory experience will provide insights on the topics covered in the classes and assigned readings. You will focus on mechanistic interpretations and reasonings of your experimental and computational measurements, followed by clearly written formal scientific reports.

Classes and assigned readings/problems will 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, acid/base catalysis, and quantitative use of substituent effects. This collection of knowledge will be 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. Please note that these approaches are not limited to organic chemistry: the ideas can be applied to structure and mechanism in any chemical sub-discipline.

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 CHM 348H, 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 to test 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 approximate and more rigorous methods in order to propose possible pathways as well as how to test each proposal. Useful theoretical overviews include intrinsic barrier theory, orbital symmetry, multidimensional energy diagrams, and no-barrier theory

<u>PREREQUISITE COURSE:</u> 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%. CHM 348H is itself a prerequisite course for <u>CHM 443HLinks to an external</u> <u>site.</u> (Physical Organic Chemistry) which covers advanced mechanistic topics (offered during the winter semester each academic year).

<u>REQUIRED TEXTBOOKS</u>: Carey & Sundberg, Advanced Organic Chemistry Part A (paperback version in the U of T Bookstore, *also available at no cost as an on-line version through the U of T Libraries; see below*). <u>Organic</u> <u>ChemistryLinks to an external site.</u> (McMurry, used in CHM 247H/CHM 249H (8th or 9th edition)) is also required.

Title:

### Advanced Organic Chemistry: Part A

Authors:

Francis A. Carey and Richard J. Sundberg

ISBN:	978038768346-1
Publisher:	Springer
Publication Date:	January 1, 2007
Туре:	Digital (URL: <u>10.1007/978-0-387-44899-2 (utoronto.ca)Links to an extern</u>

<u>CLASS SCHEDULE:</u> all classes in-person, 2:10-3:00 p.m.

Date	Tuesday	Thursday	Reading (C&S = C; McMurry= M)	(C&S chapter
September 8	Classes start Thursday	Stereochemistry , molecular mechanics, conformations	C 2.1, 2.2, 2.3	Stereochemistry , Chapter 2
13, 15	Continues	Molecular orbitals	C 1.2	Chapter 1
20, 22	Transition state theory		C 3.2	Transition state theory
27 29	Kinetics, reacti Marcus theory, energy plots, cu plots	<b>.</b>	C 3.2, 3.3, 3.6	Trends and predictions CSCh3.6
<b>October</b> 4, 6	Isotope effects	, organocatalysis	C 3.5-3.8	CSCh3 isotope effects and catalysis

11, 13	Photochemistr y	Test 1 October 13. Location: EXAM CENTRE 310	C 12.1	Chapter 12		
18, 20	Diels Alder reactions, pericyclic processes, frontier orbitals & rules		M 14 & 30, C 10.1	McMurry Ch14 Diels Alder & Ch30 pericyclic reactions		
25, 27	Nucleophilic substitution, carbocations		C 4.1, 4.3, 4.4	Chapter 4		
November 1, 3	Elimination mechanisms		C 5.10	Chapter 5		
November 7-11	Reading Week (no classes)					
15, 17	Carbanions	Carbonyl reactions	C 6.1-6.6, Decarboxylatio n	Chapter 6, Decarboxylatio n and Marcus theory		
22, 24	Carbonyl reactions, assignment information	Test 2 November 24 LOCATION: EXAM CENTER 310	C 7.1-7.3	Chapter 7		
28, <b>December</b> 1	Carbonyl reactions	Catching up	C7.4-7.7	Chapter 7		
5, 7, 8 (if needed)	Review					

<u>LABORATORY OBJECTIVES</u>: 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 26th/27th September.

## EVALUATION & GRADING SCHEMES:

There will be two available grading schemes we will use to arrive at the final reported course grade. The outcomes of both schemes will be calculated for each student, and the final reported grade will be the outcome that gives the higher mark.

## FINAL GRADE CALCULATION: SCHEME 1

- two 50-minute in-person tests during class time on Thursday 13th October and Thursday 24th November, where each test grade counts as 10% of the final grade
- a two-hour final examination, where the grade counts as **40%** of the final grade
- laboratory: attendance, observed laboratory techniques and reports as **40%** of the final grade

# FINAL GRADE CALCULATION: SCHEME 2

- two 50-minute in-person tests during class time on Thursday 13th October and Thursday 24th November, where each test grade counts as 15% of the final grade
- a two-hour final examination, where the grade counts as **30%** of the final grade
- laboratory: attendance, observed laboratory techniques and reports as **40%** of the final grade
- *submission of laboratory reports*: you are responsible for adhering to the online submission process and for meeting the stated date/time for each laboratory report. Reports will be accepted up to 48 hr. after the published due date, but a penalty of 10% of the maximum possible mark will be deducted daily for work submitted past the due date

<u>RETURN OF GRADED MATERIAL & RE-GRADING REQUESTS</u>: 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 inappropriately graded. 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.

POLICY FOR MISSED TESTS & LABORATORY SESSIONS: there are no make-up term tests in CHM 348H, and there are no make-up laboratory sessions. The policy for absence from the final examination generally allows students who petition to be offered a deferred examination if the petition is granted. Students who are absent from class for any reason (e.g. Illness or injury, family situation) and who require consideration for missed academic work must report their absence through the online absence declaration form. 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 by email to request consideration. 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, a special arrangement will be made under the principle that any alternative grading scheme is designed to reflect the work that is available for grading. *Please note that there will be no individual* supplemental opportunities to make up for a poor or missed performance on term work unless such a supplement is offered to the entire class. A student who misses a scheduled laboratory session must additionally contact Professor Dicks WITHIN ONE WEEK by email 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 any 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 discussed much more effectively in-person 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 by the instructor. 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/codebehaviour-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 <u>https://www.academicintegrity.utoronto.ca/Links to an</u> <u>external site.</u>). 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 (<u>https://uoft.me/pdt-faq (Links to an external site.</u>)).

3. Normally, students will be required to submit their course essays and tests 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 work 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: <u>https://uoft.me/pdt-faq</u>

<u>ACCESSIBILITY NEEDS</u>: students with diverse learning styles and needs are extremely 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 <u>Accessibility</u> <u>ServicesLinks to an external site</u>. as soon as possible.

<u>ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES</u>: 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 <u>Student LifeLinks to an</u> <u>external site.</u>
- full library service through <u>University of Toronto LibrariesLinks to</u> <u>an external site.</u>
- resources on conducting online research through <u>University</u> <u>Libraries ResearchLinks to an external site.</u>
- resources on academic support from the <u>Academic Success</u> <u>CentreLinks to an external site.</u>
- learner support at the Writing Centre Links to an external site.

• information for <u>Technical Support/Quercus SupportLinks to an</u> <u>external site.</u>

<u>ACKNOWLEDGEMENT OF TRADITIONAL LANDS</u>: We acknowledge that the land on which the University of Toronto operates has for thousands of years been part of the traditional lands 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.