CHM 348H (Organic Reaction Mechanisms): Fall 2023 Syllabus

Classes: Tuesdays and Thursdays 2:10-3:00 p.m., **in-person only, in the Bahen Building on St. George St. near College St., rooms BA 1220 (Tuesdays) and BA 1180 (Thursdays).**

Laboratories: Mondays or Tuesdays 8:30 a.m. - 1 p.m., starting the week of Monday 2nd October. **There is a mandatory introductory laboratory orientation session on the mornings of Monday 25th & Tuesday 26th September from 9 - 11 a.m. in room LM 108.**

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). Please request the meeting by email (r.kluger@utoronto,ca) to reserve a time. Normally available: M&F from 11:30 a.m. to 12:30 p.m. W from 1 to 2 pm. 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 request for an appointment on Wednesdays and Fridays (in-person preferred) and in-person during all scheduled laboratory hours (MT 8:30 a.m. - 1 p.m., starting on Monday 2nd October).

COURSE DESCRIPTION: 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

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%. CHM 348H is itself a prerequisite course for CHM 443H (Physical Organic Chemistry) which covers advanced mechanistic topics (offered during the winter semester each academic year).

REQUIRED TEXTBOOKS: 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*). Organic Chemistry (McMurry, used in CHM 247H/CHM 249H (8th or 9th edition)) is also required. (A free online version McMurry's 10th edition is being made available by the author): Organic Chemistry: A Tenth Edition - OpenStaxLinks to an external site.. This a gift from Professor McMurry in memory of his son, Peter.Links to an external site.

Title: **Advanced Organic Chemistry: Part A**

Authors: Francis A. Carey and Richard J. Sundberg

ISBN: 978038768346-1

Publisher: Springer

Publication Date: January 1, 2007

Type: Digital (URL: 10.1007/978-0-387-44899-2 (utoronto.ca))

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

Date	Tuesday	Thursday	Reading (C&S = C; McMurry = M)	Slide Files (C&S chapter or noted)
September 7	Classes start Thursday	Stereochemistry, molecular mechanics, conformations	C 2.1, 2.2, 2.3	Stereochemistry, Chapter 2
12, 14	Continues...	Molecular orbitals	C 1.2	Chapter 1
19, 21	Transition state theory		C 3.2	Transition state theory

26, 28	Kinetics, reaction principles, Marcus theory, linear free energy plots		C 3.2, 3.3, 3.6	Trends and predictions CSCh3.6
October 3, 5	Isotope effects, organocatalysis		C 3.5-3.8	CSCh3 isotope effects and catalysis
10, 12	Photochemistry	**Test 1 October 12. Location: EX 320**	C 12.1	Chapter 12
17, 19	Diels Alder reactions, pericyclic processes, frontier orbitals & rules		M 14 & 30, C 10.1	McMurry Ch14 Diels Alder & Ch30 pericyclic reactions
24, 26	Nucleophilic substitution, carbocations		C 4.1, 4.3, 4.4	Chapter 4
Oct 31, **November 3**	Elimination mechanisms, Carbonyl and carboxyl reactions		C 5.10	Chapter 5, Chapter 7
6-10	**Reading Week (no classes)**			

14, 16	Carboxyl Reactions, Decarboxylation	Carbanions	Chapter 7, Chapter 6	Chapter 7 Chapter 6
21, 23	Carbanions	**Test 2 November 23 LOCATION: EX 320**	Chapter 6	Chapter 6
28, 30	Heterocycles		8.6	Heterocycles
December 5, 7	Catch up & review			
Dec 11, 7 pm - 9 pm	**FINAL EXAM**	**St. Hilda's College Cartwright Hall 44 Devonshire Pl**		

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 25th/26th 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 12th October and Thursday 23rd 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 through Quercus 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

RETURN OF GRADED MATERIAL & RE-GRADING REQUESTS: laboratory reports and hour tests of the lecture material will be graded and returned to students as soon as possible. Requests for reconsideration of grading for any piece of work must be submitted as a detailed petition in writing within one week of the date in which it was available to you (even if you didn't pick it up). While some incorrect answers on tests may be given partial credit: the extent (or lack) of any partial credit is not subject to change. The request to have an error in addition of points corrected must specify the correct total or why an answer has been mis-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.

MISSED TESTS & LABORATORY SESSIONS: **there are no make-up tests in CHM 348H, and there are no make-up laboratory sessions.**

If you are absent from your studies due to illness or other reasons and unable to complete course work (e.g., a term test or a laboratory report) then a piece of written documentation is required. The following four items are the recognized forms of documentation:

- Absence Declaration via ACORN (please note the circumstances under which an absence declaration can and cannot be submitted)
- U of T Verification of Illness or Injury Form
- College Registrar's letter
- Letter of Academic Accommodation from Accessibility Services

Students who complete the ACORN Absence Declaration form and miss a laboratory session must additionally contact the laboratory coordinator, Professor Dicks (andrew.dicks@utoronto.ca) to discuss their situation within five business days of the missed laboratory. This is essential action for any consideration to be granted.

Students who complete the ACORN Absence Declaration form and miss a scheduled term test must additionally contact Professor Kluger within five business days by email (r.kluger@utoronto.ca) 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.

For extended absences and for absences due to non-medical reasons, make sure to contact your College Registrar's Office. They can help you decide between a request for an extension or other types of academic consideration.

If you suspect or know that you have a disability that is affecting your studies, learn about the services and supports available through Accessibility Services. A disability can be physical disability, sensory disability, a learning disability, mental health disorder or a short-term disability like an injury. If you are not sure whether you have a disability, you can confidentially contact Accessibility Services with your questions.

INFORMATION REGARDING USE OF ARTIFICIAL INTELLIGENCE TOOLS IN THE WRITING OF LABORATORY REPORTS

Generative Artificial Intelligence (AI) technology is evolving quickly, and it is necessary to specifically address this within the context of CHM 348H laboratory reports. AI tools such as ChatGPT (GPT stands for Generative Pre-trained Transformer) are large language models that have been trained on a limited dataset to generated content based on prompts and the data it has been trained on. **It is important to recognize there are major limitations to these tools, particularly in more specialized subjects such as chemistry.** Currently, ChatGPT and many similar models are only trained on freely available data and will not include information that is only accessible through payment, which includes much of the scholarly literature, textbooks, etc. (There is a lot of reliable information on the internet, but there is also a lot of junk, and ChatGPT does not know how to tell the difference: it has no concept whatsoever of scientific accuracy). In addition, ChatGPT does not cite its sources: when asked to include citations, it will routinely reference papers that do not exist. By using ChatGPT to generate text, you run the risk of accidentally plagiarizing one of the many sources that are included as part of its training data.

Two important learning outcomes from the laboratory component of CHM 348H are (i) development of effective scientific communication skills through written laboratory reports; and (ii) use of scientific literature to understand and evaluate experimental procedures and results. The practice and repetition of writing on your own has been shown in numerous scientific reports to lead to deeper and longer lasting learning. *In this course, the use of ChatGPT and/or other generative AI tools is permitted within the limitations of reviewing your own written work for additional suggestions of grammar, punctuation, etc.* In this manner, the tool is educational and can help you develop better writing skills when used critically and for self-analysis. **However, it is both ill-advised and prohibited to solely use these tools to attempt to write or analyze components of CHM 348H laboratory reports.** As mentioned previously, the capabilities of the systems are limited, and you will not develop the scientific communications skills needed for future studies or careers.

In summary, it is well established that these tools will misuse and fabricate information and referencing, which will be noticeable by your TAs and

laboratory instructor and will leave you susceptible to academic discipline violations (see the policy below regarding academic integrity).

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, including attendance at all examinations at the scheduled times and locations;

(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/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 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/). 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-faqLinks to an external site.).
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: https://uoft.me/pdt-faq*

ACCESSIBILITY NEEDS: 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 Accessibility Services 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 Life
- full library service through University of Toronto Libraries
- resources on conducting online research through University Libraries Research
- resources on academic support from the Academic Success Centre
- learner support at the Writing Centre
- information for Technical Support/Quercus Support

ACKNOWLEDGEMENT OF TRADITIONAL LANDS FROM TMU: "Toronto is in the 'Dish With One Spoon Territory'. The Dish With One Spoon is a treaty between the Anishinaabe, Mississaugas and Haudenosaunee that bound them to share the territory and protect the land. Subsequent Indigenous Nations and peoples, Europeans and all newcomers have been invited into this treaty in the spirit of peace, friendship and respect."

The "Dish", or sometimes it is called the "Bowl", represents what is now southern Ontario, from the Great Lakes to Quebec and from Lake Simcoe into the United States. *We all eat out of the Dish, all of us that share this territory, with only one spoon. That means we have to share the responsibility of ensuring the dish is never empty, which includes taking care of the land and the creatures we share it with. Importantly, there are no knives at the table, representing that we must keep the peace. The dish is graphically represented by the wampum pictured above.

This was a treaty made between the Anishinaabe and Haudenosaunee after the French and Indian War. Newcomers were then incorporated into it over the years, notably in 1764 with The Royal Proclamation/The Treaty of Niagara.

The land acknowledgement started in British Columbia, where there are no treaties at all. Its popularity has spread as an acknowledgment of Indigenous presence and assertion of sovereignty. It is used in a variety of ways, such as at opening events and meetings.