Chemistry
UNIVERSITY OF TORONTO

CHM443H: PHYSICAL ORGANIC CHEMISTRY

Winter 2025 Course Syllabus

I TEACHING TEAM

INSTRUCTOR, COURSE COORDINATOR
Name: Prof. Mark S. Taylor
Email: marks.taylor@utoronto.ca
Research: https://sites.chem.utoronto.ca/mst/
Office: Lash Miller, LM 622A
Student hours: T4:15–5:15 (in person, LM622A) or by appointment (online or in person)

Instructor biography (optional): BSc UofT 2000; PhD Harvard 2005; Postdoc MIT; Prof. at UofT since 2007. Research interests: organic synthesis, catalysis, physical organic chemistry

II COURSE OVERVIEW

COURSE DESCRIPTION:
The goal of the course is to acquaint you with the techniques and concepts that are used to study the mechanisms of organic reactions.

STUDENT LEARNING OUTCOMES:
By the end of this course, students will:

- understand the factors that influence rates and equilibrium constants, and how they are determined experimentally;
- understand how molecular orbital interactions influence the conformations and configurations of organic molecules;
- be familiar with concepts related to computational chemistry, including molecular mechanics, quantum chemical calculations, and basis sets;
- understand how to interpret and analyze computational results related to organic structure, reactivity and mechanism;
- understand how to use linear free energy relationships to address mechanistic questions;
- be able to derive a rate law that corresponds to a proposed mechanism, and to analyze kinetic data;
- understand how to interpret the results of kinetic isotope effect experiments;
- be able to devise experimental approaches to probe mechanisms of complex reactions;
- be able to read and understand journal articles related to modern physical organic chemistry.

PREREQUISITE COURSE(S):
This course assumes you have a solid understanding of: (i) structure, bonding, reactivity and mechanism in organic chemistry; and (ii) concepts related to

thermodynamics and kinetics. It is also assumed that you are familiar with concepts discussed in CHM348 (Organic Reaction Mechanisms), including conformational analysis, molecular orbital theory, kinetics of multistep reactions, linear free energy relationships, isotope effects).

READINGS:
Required: Course notes and recorded lectures will be posted on Quercus. Sections of the course will be based on journal articles that will be posted for you to read.
Supplemental: Modern Physical Organic Chemistry (Anslyn & Dougherty, University Science Books) is a recommended reference.

III COURSE ORGANIZATION

CHM443 consists of two lectures per week. Classes will be held in person on Mondays and Wednesdays 4–5 PM in UC261 (University College, 15 King's College Circle). Please come prepared by having done any assigned reading and printed out / downloaded the class notes posted on Quercus in advance. A second version of the notes with any annotations from the lecture will be posted afterwards. Questions are welcome during class time and after class. Lecture audio will be recorded and made available for streaming. Please be aware that reading the posted class notes or listening to the recorded lectures is not a substitute for attending classes.

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

DATES	WEEK	TOPICS
Jan 6–8	1	Introduction to course; Thermodynamics and kinetics review; Structure and bonding
Jan 13–15	2	Structure and bonding; Computational chemistry. ***Calculations begin***
Jan 20–22	3	Computational chemistry; Overview of methods for mechanistic elucidation
Jan 27–29	4	Linear free energy relationships. ***Jan 29: calculations complete***
Feb 3–5	5	Linear free energy relationships; kinetics
Feb 10–12	6	Kinetics. ***Feb 14: computational assignment due.***
Feb 17–21	–	***READING WEEK***
Feb 24–26	7	Kinetics.
Mar 3–5	8	Kinetic isotope effects. ***Mar 5: term test.***
Mar 10–12	9	Kinetic isotope effects; noncovalent interactions ***Mar 10: last day to drop S courses.*** ***Mar 10: paper selection (with instructor approval) due.***
Mar 17–19	10	Noncovalent interactions
Mar 24–26	11	Case studies ***Mar 24: Recorded presentations due.*** ***Mar 24–28 oral exams***

Mar 31–Apr 2	12	Case studies ***Mar 31–Apr 4 oral exams***

IV EVALUATION/GRADING SCHEME

OVERVIEW:
Computational assignment: 15%
Term test: 20%
Research literature analysis (recorded presentation + oral exam): 25%
Final exam: 40%

ASSESSMENT DATES & MARK BREAKDOWN:
1. Computational assignment (15% total): 5% for completing assigned calculations (due date Jan 29) plus 10% for written report (due date Feb 14 5:00 PM, electronically via PDF upload to Quercus).

2. Term Test (20%*, Wednesday March 5): 50 minutes, to be written during regularly scheduled class time.

3. Research literature analysis (25% total): Paper selection (with approval of the instructor) by Mar 10. Recorded presentations (10%) to be uploaded to Quercus by Mar 24, 5:00 PM. Oral exams (15%) will take place the weeks of Mar 24 and Mar 31.

4. Final exam (40%): during the April examination period.

*An alternative grading scheme in which the weighting of the term test will be decreased to 10% and that of the final exam increased to 50% will be evaluated for each student. For students who miss the term test with appropriate documentation, the weighting of the final exam will be increased to 60%.

V COURSE POLICIES

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

(i) professional and respectful attitude during all course activities, including classes, laboratories, tutorials, 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 (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation)
(iv) familiarity with the university policy on Academic Integrity (overleaf)

- Course website: q.utoronto.ca (in your Quercus Dashboard, click on "CHM 443H Winter 2025"). **Please check the Quercus course website regularly for**:

- general course information
- class notes
- all important announcements related to the course

- 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 443H 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 chemistry can be talked about much more effectively through student hours rather than by email, and that sending emails is not a substitute for attending classes. The student hours are posted at the Quercus course website. The instructor is also available by appointment.

Important: please do not send emails through the Quercus internal email system: the contact information for the course instructor is listed on p. 1.

- 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 a Course Instructor, I 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.

- 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 an assignment) then a piece of written documentation is required. The following four items are the recognized forms of documentation:

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

  There are no make-up term tests in CHM 443H. 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. **Students who complete the ACORN Absence Declaration form must**

additionally Prof. Taylor to discuss their situation within five business days of the missed piece of work. This is essential action for any consideration to be granted.

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 withe your questions.

- **Information Regarding Use of Artificial Intelligence Tools in the Writing of Assignments:**
  Generative Artificial Intelligence (AI) technology is evolving quickly, and it is necessary to specifically address this within the context of CHM443H assignments. 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 the limitations of 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.

- Learning outcomes of CHM443H include (i) understanding how to interpret and analyze computational results related to organic structure, reactivity and mechanism; and (ii) being able to read and understand journal articles related to modern physical organic chemistry. 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 assignments or reports. As mentioned previously, the capabilities of the systems are limited, and you

will not develop the scientific communication 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 instructor and will leave you susceptible to academic discipline violations (see the "Academic Integrity" section on p. 10 of the syllabus).

- Privacy language and appropriate use of course materials: see the syllabus "Copyright" section.

- Policy for late assignment submissions: 10% will be deducted daily for course work submitted after the posted due date. Assignments that are more than 10 days overdue will not be accepted.

- Policy for reweighting due to missed pieces of academic work. For students missing the term test for a valid reason, the weighting of the final exam will be increased to 60%.

- Requests for re-grading of term tests must be made within five business days of the posting of the answer guide. Only term tests written in pen will be eligible for re-grading.

VI TECHNOLOGY REQUIREMENTS

- This course requires the use of computers, and technical issues are possible. When working on a piece of academic work, students are responsible for scheduling enough time to allow for reasonable delays due to technical difficulties to be overcome, so such issues will not be acceptable grounds for deadline extension. Particularly, maintaining an up-to-date independent backup copy of your work is strongly recommended to guard against hard-drive failures, corrupted files, lost computers, etc.

VII INSTITUTIONAL POLICIES & SUPPORT

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 (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 assignments/presentations:

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 report. **Please note that the use of websites (such as Chegg.com) to post post/access answers to questions/assignments is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**

On quizzes and term tests:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post quiz/term test questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**
2. Looking at someone else's answers or collaborating/discussing answers during a quiz or term test.
3. Misrepresenting your identity.

In general 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 www.academicintegrity.utoronto.ca/).

Plagiarism Detection

Normally, students will be required to submit their written work 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)".

COPYRIGHT

If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited.

Audio from sections of this course, including your participation, may be recorded and will be available to students in the course for listening remotely and after each session.
Course audio recordings and materials belong to your instructor, the University, and/or other sources depending on the specific facts of each situation, and are protected by copyright. Do not download, copy, or share any course or student materials or recordings without the explicit permission of the instructor.
For questions about recording and use of audio recordings in which you may be audible, please contact your instructor.

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 an assignment, tutorial, class or laboratory session. Students must inform the 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 Quercus Support

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.