



# Chemistry

UNIVERSITY OF TORONTO

## CHM443H: PHYSICAL ORGANIC CHEMISTRY

### W2024 Course Syllabus

## I TEACHING TEAM

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### INSTRUCTOR

Name: Prof. Mark S. Taylor

Email: [marks.taylor@utoronto.ca](mailto:marks.taylor@utoronto.ca)

Research: : <https://sites.chem.utoronto.ca/mst>

Office: Lash Miller, LM 622A

Student hours (online or in person): by appointment

Instructor biography: BSc UofT 2000; PhD Harvard 2005; Postdoc MIT; Prof. at UofT since 2007. Research interests: organic synthesis, catalysis, physical organic chemistry. <https://sites.chem.utoronto.ca/mst/>

## II COURSE OVERVIEW

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### 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 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

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CHM443 consists of two lectures per week. Classes will be held in person on Mondays and Wednesdays 4–5 PM in BL112 (Claude T. Bissell building, 140 St. George Street). 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 Quercus page:** <https://q.utoronto.ca/courses/335555>

#### COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

DATES	WEEK	TOPICS
Jan 8–10	1	Introduction to course; Thermodynamics and kinetics review; Structure and bonding
Jan 15–17	2	Structure and bonding; Computational chemistry. <i>Calculations begin</i>
Jan 22–24	3	Computational chemistry; Overview of methods for mechanistic elucidation
Jan 29–31	4	Linear free energy relationships. <i>Jan 29: calculations complete</i>
Feb 5–7	5	Linear free energy relationships; kinetics
Feb 12–14	6	Kinetics. <i>Feb 12: computational assignment due.</i>
Feb 19–21	-	<b>READING WEEK</b>
Feb 26–28	7	Kinetics; kinetic isotope effects
Mar 4–6	8	Kinetic isotope effects. <i>Mar 6: term test.</i>
Mar 11–13	9	Noncovalent interactions. <i>Mar 11: last day to drop S courses.</i> <i>Mar 13: paper selection (with instructor approval) due.</i>
Mar 18–20	10	Case studies.
Mar 25–27	11	<i>Student in-class presentations, oral exams</i>
Apr 1–3	12	<i>Student in-class presentations, oral exams</i>

## **IV EVALUATION/GRADING SCHEME**

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### **OVERVIEW:**

Computational assignment: 15%

Term test: 20%

Research literature analysis (in-class 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 12 4:00 PM, electronically via PDF upload to Quercus).

2. Term Test (20%\*, Wednesday March 6): 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 13. Student presentations (10%, during class time) and oral exams (15%, to be scheduled outside of class time) will take place Mar 25/27 and Apr 1/3.

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**

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- Each member of this course is expected to maintain a:
  - (i) professional and respectful attitude during all course activities, including classes, student hours 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)
- 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

Students who complete the ACORN Absence Declaration form must additionally contact me 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 with your questions.

- Use of Generative AI in CHM443. Students may not use artificial intelligence tools for taking tests or completing course assignments. However, these tools may be useful when gathering information from across sources and assimilating it for understanding. Representing as one's own an idea, or expression of an idea, that was AI-generated may be considered an academic offense in this course.
- Communication with instructor: emails regarding course content or logistics are welcome. Please use your UofT email address, and do not send messages

via Quercus. I will respond to emails within 24 hrs. on weekdays whenever possible.

- Privacy and appropriate use of course materials: please 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. Due to the timing of the in-class presentations, rescheduling will not be possible. Students who miss the in-class presentation for a valid reason will give a 10-minute presentation to the instructor immediately prior to their oral examination.
- 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%.
- Assignment submission methods: the computational report is to be submitted electronically (PDF only) via Quercus.
- Process for requesting re-grading of course work: only term tests written in pen will be eligible for re-grading.

## **VI TECHNOLOGY REQUIREMENTS**

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- 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**

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### **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](http://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 written work:

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 assignment material/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.**

On term tests and exams:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com) to post 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 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/](http://www.academicintegrity.utoronto.ca/)).

## **COPYRIGHT**

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

Lecture audio will be recorded, and the recordings made available for streaming via Quercus. Students may also create their own recordings of the lecture audio if they wish. Recordings are intended to permit lecture content review so as to enhance understanding of the topics presented. Audio recordings are not substitutes for attending class.

Students should note that their voice may be recorded as part of the lecture audio. Please speak to the instructor if this is a concern for you.

In accordance with the Accessibility for Ontarians with Disabilities Act, 2005, persons who have special needs will be accommodated.

Students agree to the following terms when creating or using audio recordings of lectures:

- Recordings are not to be distributed without the permission of the instructor via the Internet, using social media such as Facebook, peer-to-peer file sharing such as One Drive or Dropbox, or other distribution channels.
- Recordings are not to be shared with other classmates unless they are to be used in collaborative assignments, or if the instructor permits for other reasons.

Non-compliance with these terms violates an instructor's intellectual property rights and the Canadian Copyright Act. Students violating this agreement will be subject to disciplinary actions under the Code of Student Conduct.

### **ACCESSIBILITY NEEDS**

Students with diverse learning styles and needs are welcome in CHM443H. 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 or class. 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.