

CHM 443HS: Physical Organic Chemistry

Course Syllabus: Winter 2023

I CONTACTS



INSTRUCTOR

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Office: LM-Davenport wing (Rm 462)

Online student hours: MW (5pm ET)

Classes

Classes: MW 4-5pm ET (LM157)

II COURSE OVERVIEW

COURSE DESCRIPTION:

The purpose of this course is to familiarize students with the tools of mechanistic organic chemistry. Topics include kinetics and mechanisms, transition state theory, kinetic isotope effect, molecular modelling and computational chemistry, pH-rate profile, Hammett equation, Brönsted equation, Marcus equation, reactivity-selectivity principle, and reaction energetics. These methods of analyzing reaction mechanisms will be applied to a variety of reactions including stereoselective organocatalysis, transition metal-based catalysis, and pericyclic reactions. Fundamental concepts discussed in this course is also applicable to bioorganic and bioinorganic chemistry.

STUDENT LEARNING OUTCOMES:

By the end of this course, students will learn a variety skills to probe organic reaction mechanisms.

- Learn how to evaluate reaction mechanisms using physical organic chemistry tools including kinetic analysis, LFER, and pH-rate profiles.
- Read mechanistic organic chemistry papers critically and provide written and oral presentations clearly.
- Understand experimental and computational techniques to develop organocatalysts for a variety of chemical reactions.
- How to synthesize drugs with organocatalysts

PREREQUISITE COURSE:

CHM220H/CHM222H/CHM225Y, CHM348H

Textbook: Reference Anslyn and Dougherty 'Modern Physical Organic Chemistry'**III COURSE ORGANIZATION**

This course will be given in class with the following schedule.

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

- 1) 2021-Chemistry Nobel lectures (Benjamin List, David MacMillan)
- 2) Basic Kinetics
- 3) Transition state theory
- 4) Topics in Computational Chemistry (molecular modelling)
- 5) LFER (Linear Free Energy Relationship)
- 6) Brønsted Equation and pH-rate profiles
- 7) Reactivity Selectivity Principle
- 8) Marcus equation
- 9) 2-D Energy diagram (William Jencks)
- 10) Reaction Progress Kinetic Analysis (Donna Blackmond)
- 11) Kinetic isotope effect
- 12) Organocatalysis (fundamentals to applications)

IV EVALUATION/GRADING SCHEME

Important: if an unexpected technical issue occurs with a university system (e.g., Quercus services, network outage) that affects availability or functionality, it may be necessary to revise the timing or weighting of the assessments.

1) Computational assignment	20%
2) Midterm	20% or 30%
3) Final exam	<u>50% or 60%</u>
4) Total	100%

FINAL ASSESSMENT

There will be a Final Assessment Period in April

IV 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)
- 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.
- Communication with instructor (e.g., I will respond to email within 24 hrs. on weekdays).
- Privacy language and appropriate use of course materials:
<https://teaching.utoronto.ca/ed-tech/audio-video/sample-statements/>

V TECHNOLOGY REQUIREMENTS

Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here:

<https://www.vicereprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/>

Advice for students more broadly regarding online learning is available here:

<https://onlinelearning.utoronto.ca/getting-ready-for-online/>

This course requires the use of computers, and of course sometimes things can go wrong when using them. You are responsible for ensuring that you maintain regular backup copies of your files, use antivirus software (if using your own computer), and schedule enough time when completing an assignment to allow for delays due to technical difficulties. Computer viruses, crashed hard drives, broken printers, lost or corrupted files, incompatible file formats, and similar mishaps are common issues when using technology, and are not acceptable grounds for a deadline extension.

VI INSTITUTIONAL POLICIES AND SUPPORT

ACADEMIC INTEGRITY

On 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:

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 <https://www.academicintegrity.utoronto.ca/>).

Use of Turnitin

"Normally, students will be required to submit their course essays to Turnitin.com 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 Turnitin.com reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of the Turnitin.com service are described on the Turnitin.com web site".

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. More information regarding this is available here: <https://teaching.utoronto.ca/ed-tech/audio-video/copyright-considerations/>

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 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 and 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

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.