

CHM 1003: PHYSICAL ORGANIC CHEMISTRY, WINTER 2021

I CONTACTS



INSTRUCTOR

Prof. Mark S. Taylor

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Online student hours: Friday 3–4 PM or by appointment

B.Sc. (Toronto, 2000), Ph.D. (Harvard, 2005) Postdoc (MIT). Professor at U of T 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;
- identify different types of noncovalent interactions and understand how they can be probed experimentally;
- 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;
- understand how to use linear free energy relationships to address mechanistic questions;
- 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 HOW THE COURSE IS ORGANIZED

Course delivery will be through a combination of pre-recorded lectures and 'live' online sessions. Students are expected to view the pre-recorded lectures prior to the online sessions, which will be used primarily for Q&A, problem-solving and discussion of examples.

Online sessions will be held on Mondays and Wednesdays, 4:10–5 PM, via Zoom.

Because some of the content will be delivered asynchronously via pre-recorded lectures, we may not use the full 100 min each week.

TENTATIVE LIST OF TOPICS:

| UNIT | TOPICS | Relevant chapters from Anslyn/Dougherty |
|------|--|---|
| 1 | Thermodynamics, kinetics and potential energy surfaces. Experimental determination of quantities related to thermodynamics and kinetics. | 2, 7 |
| 2 | Structure and bonding. Basics of MO theory. Hyperconjugation and anomeric effects. Introduction to computational chemistry. | 1, 2, 14 |
| 3 | Noncovalent interactions. Ionic interactions, hydrogen bonding, interactions of aromatics, halogen and chalcogen bonding, hydrophobic effects. Assignment 1 due 11:59 PM, Feb 3 | 3 |
| 4 | What is a mechanism? Overview of tools for elucidation of mechanism. | 7, 8 |
| 5 | Kinetics. Derivation of rate laws. Classical kinetics versus reaction progress kinetic analysis. Assignment 2 due 11:59 PM, Feb 24 | 7 |
| 6 | Isotope effects. Deuterium kinetic isotope effects (primary and secondary). Heavy atom kinetic isotope effects. Assignment 3 due 11:59 PM, Mar 10 | 8 |
| 7 | Linear free energy relationships. Hammett σ constants. Steric parameters. Solvent parameters. LFERs based on calculated quantities. Assignment 4 due 11:59 PM, Mar 24 | 8 |
| 8 | Case studies. Examples from the primary research literature. | |

IV EVALUATION/GRADING SCHEME

ASSIGNMENTS (four in total) worth 12.5% each

PRESENTATION 15% + ORAL EXAM 10% (presentations to take place Mar 29/31, with oral exams the week of Apr 5/7)

FINAL WRITTEN ASSIGNMENT 25% (due during the final assessment period, Apr 21 11:59 PM)

MARK BREAKDOWN

Assignments $4 \times 12.5\% = 50\%$ total grade

Presentation, oral exam = 25% total grade

Final written assignment = 25% total grade

Note: it may be necessary to revise the timing or weighting of the assessments.

FINAL ASSESSMENT

Instead of an exam-style final assessment, a final written assignment (worth 25% of the final grade – see above) will be due during the April assessment period.

V COURSE POLICIES

E-mail: I am happy to respond to course-related e-mail inquiries. Please include the course code CHM1003 in the title of your e-mail, and use your UTOR e-mail account to send the message. Normally, I'll get back to you within 24 hours during the week. However, e-mail is not an alternative to participating in virtual student hours, nor is it a mechanism for lengthy discussions or to explain material that was covered in lectures you missed.

Participation: Your participation in the online discussion sessions is highly encouraged, including through audio or by typing in the chat. Please be mindful to communicate in a civil and respectful way so that all students feel comfortable in sharing their questions and ideas. University statement regarding a positive learning environment: *“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. U of T does not condone discrimination or harassment against any persons or communities.”*

Privacy: This course, including your participation, will be recorded on video and will be available to students in the course for viewing remotely and after each session.

Course videos 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 videos without the explicit permission of the instructor.

For questions about recording and use of videos in which you appear, please contact me.

Due dates/penalties for late work: Assignments are due (via Quercus) at 11:59 PM on the dates indicated in Section III. Penalty for late submissions: 10% of the mark per day late. Please follow all instructions regarding acceptable file formats.

VI TECHNOLOGY REQUIREMENTS

Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here: <https://www.viceprovoststudents.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.

VII 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:

In papers and assignments:

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.

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/>).

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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.

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](#)