

SYLLABUS

CHEM 311 / ENCH 311 Mechanistic Organic Chemistry

Fall, 2021

Chernoff Hall, Rm 117: Mon 8:30 AM, Wed 10:30 AM, Fri 9:30 AM

Instructor: Prof. Graeme Howe

Instructor Contact Information:

Chernoff Hall, Rm 512, Ph: (613) 533-6089, email: graeme.howe@queensu.ca

Office Hours: By appointment

TA: Carolyn Kimball

TA Contact Information: Email: c.kimball@queensu.ca

Tutorials: Mon 6:30 PM, Virtual; Wed 11:30 AM, Chernoff Hall Rm 211

Office Hours: by appointment

By the end of this course, students will be able to:

1. Apply models of molecular orbitals and hybridization to predict the structures and properties of chemicals.
2. Apply models of conjugated systems and aromaticity to predict the products of pericyclic reactions.
3. Correlate changes in chemical structure with changes in transition states using one- and two-dimensional reaction coordinates.
4. Use kinetic isotope effects, solvent effects, and linear free energy relationships as tools to evaluate mechanisms of organic reactions.
5. Predict the reactivity of non-classical carbocations and various ion pairs.
6. Rationalize the regiochemistry, stereochemistry, and reactivity of various classes of reactions.
7. Apply general chemical principles to predict or understand the structure and reactivity of molecules.

Supplemental texts

Modern Physical Organic Chemistry (Anslyn and Dougherty) is a particularly useful text that is easily digestible. *Advanced Organic Chemistry* by Carey and Sundberg is another useful resource. An electronic version of this text is freely available through the Queen's Library.

Course Outline

Supplemental chapters from Anslyn & Dougherty are given in parentheses

- **Structure and models of bonding** (1.1) – Basics of bonding, VSEPR and hybridization, valence bond theory, hybridization indices
- **Thermochemistry of stable molecules and reactive intermediates** (2.1, 2.2) – Thermodynamics, thermochemistry of reactive intermediates, carbanions, carbocations, radicals
- **Hückel molecular orbital theory applied to p systems** (14.2, 14.3, 14.5) – Hückel MO theory, Frost circles, aromaticity/antiaromaticity, Semiempirical MO methods
- **Reactivity, kinetics, and mechanisms** (7.3, 7.8) – Transition state theory, kinetic postulates, More O'Ferrall-Jencks plots
- **Experiments related to thermodynamics and kinetics** (8) – experimental considerations, isotope effects, linear free energy relationships, substituent effects, Hammett plots, Taft equation, Swain-Scott parameters, Grunwald-Winstein relationship, solvent effects

- **Catalysis** (9.1 – 9.3) – General principles, forms of catalysis, acid-base catalysis, Brønsted relationship
- **Thermal pericyclic reactions** (15.2 – 15.5) – Cycloaddition reactions, electrocyclic reactions, sigmatropic reactions
- **Organic reaction mechanisms – Substitutions** (10.18, 10.19, 11.5) – Aliphatic substitution, structure-function correlations, carbocation rearrangements, anchimeric assistance, non-classical carbocations, electrophilic aromatic substitution, nucleophilic aromatic substitution
- **Organic reaction mechanisms – Eliminations** (10.12, 10.13) – Elimination vs. substitution, E1cB mechanisms, structure-function correlations, regiochemical considerations, carbonyl-forming reactions
- **Organic reaction mechanisms - Carbonyl chemistry** (10.8, 10.17, 11.1) – Keto-enol tautomerism, enols and enolates, nucleophilic carbonyl additions, acyl transfer reactions, substitution reactions of acid derivatives, intramolecular catalysis
- **Organic reaction mechanisms – Selected case studies from primary research literature**
- **Photochemistry** – (16.1 – 16.3; time permitting) Jablonski diagrams, fluorescence, phosphorescence, bimolecular photophysical processes, photochemical reactions

Delivery of course material

Every effort will be made to record the lectures and make them available via the course website. Pre-recorded videos intended to supplement lectures will be made available through the course website, but these videos are not required viewing.

Grading Scheme

- Midterm (Date/Time: **TBD**): 1 x 30%
- Problem sets: 4 x 5%
- Final Exam: 45%
- Tutorial Quizzes: 5%

Assessments

Problem sets, the midterm and the final exam will be released via onQ at a set time and date and must be turned in prior to the **strict** deadline. TurnItIn will be used to check all materials for plagiarism prior to grading. All assessed work must be entirely your own, and a zero-tolerance policy will be enforced for academic dishonesty.

Tutorials:

There are two CHEM311/ENCH311 tutorial sections: a virtual section held live over Microsoft Teams, and an in-person tutorial held in Chernoff 211 (see course website for Teams Meeting info). Students must log into the tutorial on time, as the Teams Meeting will be locked to new attendees 15 minutes after the scheduled start time. Similarly, students who are more than 15 minutes late to the in-person tutorial will not be permitted to write that week's quiz (see below).

At the end of each tutorial, there will be a short quiz. For each quiz, you will receive a 5 for getting it correct, a 3 for taking it, or a 0 for missing it. If you are not logged into the tutorial in Microsoft Teams when the tutorial ends, you will receive a 0 for the quiz.

Grading Method

All components of this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to Queen's Official Grade Conversion Scale:

Queen's Official Grade Conversion Scale

Grade	Numerical Course Average (Range)
A+	90-100
A	85-89
A-	80-84
B+	77-79
B	73-76
B-	70-72
C+	67-69
C	63-66
C-	60-62
D+	57-59
D	53-56
D-	50-52
F	49 and below

Timing of Final Examinations

The exam dates for each Term are listed on the Faculty of Arts and Science webpage under "[Important Dates](#)." Student exam schedules for the Fall Term are posted via SOLUS immediately prior to the Thanksgiving holiday; for the Winter Term they are posted on the Friday before Reading Week, and for the Summer Term they are individually noted on the Arts and Science Online syllabi. **Students should delay finalizing any travel plans until after the examination schedule has been posted. Exams will not be moved or deferred to accommodate employment, travel/holiday plans or flight reservations.**

Remote Exams

For exams being offered remotely, Regulation 7.2.3. [Restrictions on Assessment](#) is waived. Remote exams will be allowed in the last two weeks of classes and in the study period designated by Senate prior to the examination period in order to accommodate the limited number of online proctoring seats available.

Academic Integrity

Queen's students, faculty, administrators and staff all have responsibilities for upholding the fundamental values of academic integrity; honesty, trust, fairness, respect, responsibility and courage (see www.academicintegrity.org). These values are central to the building, nurturing and sustaining of an academic community in which all members of the community will thrive. Adherence to the values expressed through academic integrity forms a foundation for the "freedom of inquiry and exchange of ideas" essential to the intellectual life of the University (see the Senate Report on Principles and Priorities <http://www.queensu.ca/secretariat/policies/senate/report-principles-and-priorities>).

Students are responsible for familiarizing themselves with the regulations concerning academic integrity and for ensuring that their assignments and their behaviour conform to the principles of academic integrity. Information on academic integrity is available in the Arts and Science Calendar (see Academic Regulation 1 <http://www.queensu.ca/artsci/academic-calendars/regulations/academic-regulations/regulation-1>), on the Arts and Science website (see <https://www.queensu.ca/artsci/students-at-queens/academic-integrity>), and from the instructor of this course. Departures from academic integrity include plagiarism, use of unauthorized materials, facilitation, forgery and falsification, and are antithetical to the development of an academic community at Queen's. Given the seriousness of these matters, actions which contravene the regulation on academic integrity carry sanctions that can range from a warning or the loss of grades on an assignment to the failure of a course to a requirement to withdraw from the university.

Calculator Policy

As noted in Academic Regulation 9.2, "Calculators acceptable for use during quizzes, tests and examinations are intended to support the basic calculating functions required by most Arts and Science courses. For this purpose, the use of the **Casio 991 series calculator** is permitted and is the only approved calculator for Arts and Science students."

Technology

Web Browsers – onQ performs best when using the most recent version of the web browsers, Chrome or Firefox. Safari and Edge are strongly discouraged as these web browsers are known to cause issues with onQ.

Internet Speed – While wired internet connection is encouraged, we recognize that students may be relying on a wireless connection. A minimum download speed of 10 Mbps and up to 20 Mbps for multimedia is recommended. To test your internet speed, <https://www.speedtest.net/>

For technology support ranging from setting up your device, issues with onQ to installing software, contact ITS Support Centre <https://www.queensu.ca/its/itsc>

Copyright of Course Materials

Course materials created by the course instructor, including all slides, presentations, handouts, tests, exams, and other similar course materials, are the intellectual property of the instructor. It is a departure from academic integrity to distribute, publicly post, sell or otherwise disseminate an instructor's course materials or to provide an instructor's course materials to anyone else for distribution, posting, sale or other means of dissemination, without the instructor's *express consent*. A student who engages in such conduct may be subject to penalty for a departure from academic integrity and may also face adverse legal consequences for infringement of intellectual property rights.

Notice of Recording

Synchronous (live) classes will be delivered in this course via in-person delivery and through a video conferencing platform supported by the University [MS Teams, Zoom]. Steps have been taken by the University to configure these platforms in a secure manner. Classes will be recorded with video and audio (and in some cases transcription) and will be made available to students in the course for the duration of the term. The recordings may capture your name, image or voice through the video and audio recordings. By attending these live classes, you are consenting to the collection of this information for the purposes of administering the class and associated coursework. If you are concerned about the collection of your

name and other personal information in the class, please contact the course instructor to identify possible alternatives.

To learn more about how your personal information is collected, used and disclosed by Queen's University, please see the general [Notice of Collection, Use and Disclosure of Personal Information](#).

Acknowledgement of Territory

Queen's University is situated on traditional [Anishinaabe and Haudenosaunee Territory](#).

Accommodations for Disabilities

Queen's University is committed to achieving full accessibility for people with disabilities. Part of this commitment includes arranging academic accommodations for students with disabilities to ensure they have an equitable opportunity to participate in all of their academic activities. The Senate Policy for Accommodations for Students with Disabilities was approved at Senate in November 2016 (see <https://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslclwww/files/files/policies/senateandtrustees/ACADACCOMMPOLICY2016.pdf>). If you are a student with a disability and think you may need academic accommodations, you are strongly encouraged to contact the **Queen's Student Accessibility Services (QSAS)** and register as early as possible. For more information, including important deadlines, please visit the QSAS website at: <http://www.queensu.ca/studentwellness/accessibility-services/>

Academic Considerations for Students in Extenuating Circumstances

Queen's University is committed to providing academic consideration to students experiencing extenuating circumstances that are beyond their control and are interfering with their ability to complete academic requirements related to a course for a short period of time. The Senate Policy on Academic Consideration for Students in Extenuating Circumstances is available at <http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslclwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf>

Each Faculty has developed a protocol to provide a consistent and equitable approach in dealing with requests for academic consideration for students facing extenuating circumstances. Arts and Science undergraduate students can find the Faculty of Arts and Science protocol and the portal where a request can be submitted at: <http://www.queensu.ca/artsci/accommodations>. Students in other Faculties and Schools who are enrolled in this course should refer to the protocol for their home Faculty.

If you need to request academic consideration for this course, you will be required to provide the name and email address of the instructor/coordinator. Please use the following:

Instructor Name: Prof. Graeme Howe

Instructor Email Address: graeme.howe@queensu.ca

Discussion Guidelines

University is a place to share, question and challenge ideas. Each student brings a different lived experience from which to draw upon. To help one another learn the most we can from this experience please consider the following guidelines.

1. Make a personal commitment to learn about, understand, and support your peers.

2. Assume the best of others and expect the best of them.
3. Acknowledge the impact of oppression on the lives of other people and make sure your writing is respectful and inclusive.
4. Recognize and value the experiences, abilities, and knowledge each person brings.
5. Pay close attention to what your peers write before you respond. Think through and re-read your writings before you post or send them to others.
6. It's ok to disagree with ideas, but do not make personal attacks.
7. Be open to being challenged or confronted on your ideas and to challenging others with the intent of facilitating growth. Do not demean or embarrass others.
8. Encourage others to develop and share their ideas.