

CHEM 212 / ENCH 212
Principles of Chemical Reactivity

Fall, 2022

Biosciences Complex, Biosci 1102: Mon 11:30 AM, Tue 1:30 PM, Thu 12:30 PM

Course Instructor: Dr. Graeme Howe
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Office hours:
Mon 2:30 – 3:30PM; Chernoff Rm 515
Thu 2:30 – 3:30PM; Chernoff Rm 515

Lab Instructor: Dr. Igor Kozin
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Lectures:	Monday, 11:30AM – 12:20PM	Biosciences Complex, Room 1102
	Tuesday, 1:30PM – 2:20PM	Biosciences Complex, Room 1102
	Thursday, 12:30PM – 1:20PM	Biosciences Complex, Room 1102

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

1. Identify reactive sites in reagents
2. Determine rate laws for simple chemical processes
3. Articulate the meaning of transition state theory and associated activation parameters
4. Predict and rationalize the effect of solvent effects and electronic effects on reactivity
5. Use experimental data obtained in the laboratory to study reaction kinetics
6. Critically analyze and communicate scientific results

Assessment of learning outcomes:

Tutorials will assess outcomes 1, 2, 3, and 4

Mid-term exam will assess outcomes 1 and 4

Final exam will assess outcomes 1, 2, 3, and 4

Labs will assess outcomes 5 and 6

Required textbook:

Organic Chemistry, Jonathan Clayden, Nick Greeves, and Stuart Warren, Oxford University Press, 2nd edition

Supplemental textbook:

Atkins' *Physical Chemistry*, Peter Atkins, Julio de Paula, and James Keeler, Oxford University Press, 11th edition

Course Outline

Recommended readings from Clayden or Atkins are given in parentheses

Section 1: Chemical Reactivity – The Basics

- a. General description of reactions: Substitution and elimination reactions (Clayden, p. 328 – 329, p. 382 – 384)
- b. Visualizing reaction mechanisms (Clayden, p. 116 – 124)

- c. Energy profiles and potential energy surfaces (Clayden, p. 250 – 252)
- d. Concepts of molecular encounters (Clayden, p. 107 – 115)

Section 2: Nucleophilic Substitution Reactions

- a. Structure-reactivity relationships (Clayden, p. 332 – 340, p. 344 – 349, p. 351 – 359)
- b. Stereochemical outcomes of substitution reactions (Clayden, p. 343 – 344)

Section 3: How Fast Do Chemical Reactions Go?

- a. Rate laws and rate constants: 1st and 2nd order substitution reactions (SN1 and SN2), (Clayden, p. 257 – 262, p. 328 – 332; Atkins Section 20A.2, Section 20E)
- b. Kinetics of consecutive elementary reactions (Atkins Section 20E.3, 20E.4, 20E.5)
- c. Temperature dependence of rate constants (Atkins Section 20D)
- d. Measuring rate constants (Atkins Section 20B)

Section 4: Elimination Reactions

- a. General description of E1 and E2 reactions (Clayden, p. 382 – 387)
- b. Elimination vs. substitution (Clayden, p. 384 – 391)
- c. Regiochemical and stereochemical outcomes in elimination reactions (Clayden, p. 391 – 399)
- d. The E1cb reaction (Clayden, p. 399 – 404)

Section 5: Electrophilic Aromatic Substitution Reactions

- a. General description of EAS reactions (Clayden, p. 471 – 478)
- b. Reactions of substituted benzenes (Clayden, p. 479 – 492)

Section 6: Reaction Dynamics

- a. Collision theory (Atkins Section 1B, Section 21A.1)
- b. Diffusion-controlled reactions (Atkins Section 21B.1)
- c. Transition state theory (Atkins Section 21C.1, 21C.2, Clayden p. 251 – 253)

Supplemental Readings

The following chapters serve as useful introductory and supplemental material for CHEM 212. You do not need to read everything listed below, but the materials listed here may help you to feel more comfortable with certain concepts that are presented in lecture. If you feel like some chemical concepts presented in lecture could use more fleshing out, these chapters may help!

- **Chapter 1:** What is organic chemistry? (an interesting read)
- **Chapter 2:** Organic structures (Good for learning how to draw organic structures efficiently)
- **Chapter 4:** Structure of molecules (useful for learning how atomic orbitals combine to form molecular orbitals)
- **Chapter 5:** Organic reactions (very useful for understand the art of curly arrow drawing)
- **Chapter 8:** Acidity, basicity, and pKas (very good for understanding what pKa values indicate, as well as how to understand/predict how pKa values will change with the structure of a molecule)

Useful Resources:

- <https://mechanisms.edu.rsc.org/> - free online tool from the Royal Society of Chemistry providing many worked examples of curly arrow mechanisms
- Several chemical reactions have been animated and can be view at <http://www.chemtube3d.com/>
- Data processing associated with the lab component of the course will require the use of Microsoft Excel

Problem Sets:

Practice problems and solutions will be posted on the CHEM/ENCH 212 OnQ site. These are not marked, but it is highly recommended that you complete these problems in preparation for the mid-term and final exams.

Tutorials:

Tutorials begin the week of September 12th, 2022.

Each tutorial will be accompanied by a pre-tutorial assignment that will be posted to onQ. While these will not be graded, you must submit your assignment to the TA *before* the start of the tutorial to receive participation credit. The tutorial will include a discussion of the assignment that is intended to clarify challenging concepts and provide an opportunity to ask questions related to said assignment. The TA will then administer a short quiz that you must complete and submit during the tutorial. Tutorials are worth 10% of your final grade, and only your 8 highest quiz grades will be used towards this 10%.

Be sure to attend the time and section that you selected when enrolling in the course.

Labs:

All labs must be attended as scheduled. All students *must* attend the introductory lab (lab group assignment, lab safety, lab quiz) in week 2 (September 13th – 15th) (~1hr)

Regular 3hr labs will be held on alternate weeks in room CHE210 on the 2nd floor of Chernoff Hall (see schedule in OnQ)

In weeks 3 – 12, students will rotate between the following 6 experiments:

- **Experiment 1: Kinetics of Nucleophilic Substitution (S_N1 Reaction Kinetics)**
- **Experiment 2: Alkaline Hydrolysis of Ethyl Acetate (S_N2 Reaction Kinetics)**
- **Experiment 3: Photo-isomerization Kinetics of 4-Hydroxyazobenzene**
- **Experiment 4: Stopped-Flow Kinetics – Reaction of Fe³⁺ and SCN⁻ Ions**
- **Experiment 5: Enzyme-Catalyzed Oxidation of DOPA**
- **Experiment 6: Gas Viscosity – Determination of Collision Cross Section for Gases**

To pass the lab component, students will be required to perform and pass 5 of the 6 listed above experiments, in accordance with the experiment schedule specific to individual lab groups. The lab schedule is printed in the CHEM/ENCH 212 Laboratory Manual and can be also accessed from the onQ course site.

Grading Scheme

- Midterm (2 hours; Date/Time: **TBD**): 25%
- Final Exam (3 hours; Date/Time: **TBD**): 40%
- Tutorial Quizzes: 10%
- Labs: 25% (Lab administration details, assessment guidelines and individual lab marking schemes are printed in the CHEM/ENCH 212 Lab Manual)

IMPORTANT:

1. Students must pass BOTH the lecture and the laboratory components to pass the course. If a student does not pass both the laboratory and lecture components of this course, they will fail the entire course and receive an overall mark of 47% or their actual mark, whichever is lower.
2. The lecture hall is equipped with lecture capturing capabilities. Every effort will be taken to record the live lecture, and this recording will be uploaded to the onQ page within 24 hours of the lecture. Attendance at the live lecture is strongly encouraged, as technical problems may impede the recording or uploading of the lecture.

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.**

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.