

**CHEM 212 / ENCH 212**  
**Principles of Chemical Reactivity**  
Fall, 2024

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**Lectures:** Lectures are delivered in person, full attendance by students is mandatory and expected.

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

1. Identify reactive sites in chemical compounds.
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 role that solvent effects and electronic effects have on chemical reactivity.
5. Collect and interpret 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, 2, 3, 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, 2<sup>nd</sup> edition.

**Supplemental textbook:**

Atkins' *Physical Chemistry*, Peter Atkins, Julio de Paula, and James Keeler, Oxford University Press, 11<sup>th</sup> edition. Older versions of this textbook can be used and will contain similar info, in similar locations.

**Course Outline**

Recommended readings from Clayden or Atkins are given in parentheses.

**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)

**Nucleophilic Substitution Reactions (Clayden Chapter 15)**

- a. Structure-reactivity relationships (Clayden, p. 332–340, p. 344–349, p. 351–359)

- b. Stereochemical outcomes of substitution reactions (Clayden, p. 343–344)

#### **Kinetics - How Fast Do Chemical Reactions Go?**

- a. Rate laws and rate constants: 1<sup>st</sup>- and 2<sup>nd</sup>-order substitution reactions ( $S_N1$  and  $S_N2$ ), (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)

#### **Elimination Reactions (Clayden Chapter 17)**

- 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 E1<sub>cb</sub> reaction (Clayden, p. 399–404)

#### **Electrophilic Aromatic Substitution Reactions (Clayden Chapter 21)**

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

#### **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)

#### **Nucleophilic Aromatic Substitution Reactions (Clayden in Chapter 22, p. 514–527)**

#### **Enzyme Catalysis (Atkins Section ~20H) – if time permits**

#### **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!

#### **Organic Chemistry by Clayden, 2<sup>nd</sup> Edition**

- **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 understanding the art of curly arrow drawing)
- **Chapter 8:** Acidity, basicity, and pKa (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 <https://www.chemtube3d.com/>
- Data processing associated with the lab component of the course will require the use of Microsoft Excel.

### **Tutorial Problem Sets/Tutorial Assignments/Tutorial Quizzes**

Tutorial Problem Sets and Tutorial Assignments will be posted in advance on the CHEM/ENCH 212 OnQ site. Try to work through all the practice problems before attending the Tutorial. These are not marked, but it is highly recommended that you complete these problems in preparation for the mid-term and final exams. TAs will go over these practice problems each week during the tutorials. Practice Quizzes will also be delivered in the tutorials. **These items will not be graded, however, your mandatory attendance during the tutorials will be graded (10% of course grade).** The solutions to the Problem Sets and Assignments will be posted on onQ after all sections have worked through the material.

### **Tutorials**

**Tutorials are mandatory** and you will be given an attendance mark. There are 11 tutorials, but you can miss 2 without penalty (by universal design for learning). In onQ, the calculation will drop your lowest 2 grades of the 11. **NO EXCEPTIONS, NO CHANGES WILL BE MADE TO THE POLICY. ALL ABSENCES WILL BE ENTERED AS ZERO REGARDLESS OF THE SITUATION.** Tutorial attendance will count towards 10% of your final grade in the course, so please make sure you attend at least 9/11 tutorial sessions for full marks.

Tutorials begin **September 11/13, 2024** depending on your TUTORIAL section. **MAKE SURE TO ATTEND YOUR PROPER TUTORIAL SECTION TO OBTAIN THE FULL ATTENDANCE MARKS.**

The tutorial TAs will go over Problem Sets/Assignments to clarify challenging concepts and provide an opportunity to ask questions about course topics. They will also administer very short Practice Quizzes to help you prepare for exams. Attendance in the 11 Tutorials is worth 10% of your final grade (we will drop the lowest two tutorial attendance grades). Be sure to attend the proper Tutorial section (check Solus).

### **Labs:**

All labs must be attended as scheduled. **All students *must* attend the introductory lab (lab group organization, lab safety, lab quiz).** Students will be organized in Pools and given a lab group number (for you and your lab partner). After the Introductory Lab, regular 3-hr labs will be held on alternate weeks (please see schedule posted on OnQ).

Students will rotate between the following 6 experiments (depending on lab group #):

- **Experiment 1: Kinetics of Nucleophilic Substitution ( $S_N1$  Reaction Kinetics)**
- **Experiment 2: Alkaline Hydrolysis of Ethyl Acetate (Second-order Reaction Kinetics)**
- **Experiment 3: Photo-isomerization Kinetics of 4-Hydroxyazobenzene**
- **Experiment 4: Stopped-Flow Kinetics – Reaction of  $Fe^{3+}$  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. Students repeating the course should request a laboratory exemption, and if not granted, will work alone in the lab.

### Grading Scheme

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

**There are NO MAKE-UP EXAMS in CHEM 212/ENCH 212. Please report Midterm conflicts well in advance to your Instructor for approval; your final exam will be worth more to compensate. For example, if you have advance permission to miss the Midterm from your Instructor, your final exam will then be worth 65% instead of 40%. NO EXCEPTIONS, NO RE-WRITES.**

### IMPORTANT:

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.

### 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](http://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.

### **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:** Dr. Jason Z. Vlahakis

**Instructor Email Address:** [vlahakis@queensu.ca](mailto:vlahakis@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.