SYLLABUS 2019 CHEM/ENCH 212: Principles of Chemical Reactivity

Course instructor: Dr Avena Ross
CHE 407, Chernoff Hall
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Office hours are in rm 515 Chernoff Hall:
Mondays 2:30 pm-3:30 pm
Thursdays 9:30 am-10:30 am

Lab instructor: Dr Igor Kozin
CHE 124, Chernoff Hall
phone: 613-533-6000 ext 74665
email: igor.kozin@chem.queensu.ca

CHEM/ENCH 212 is taught using OnQ

Lectures: Mondays 1:30 pm-2:20 pm, in Etherington Aud.
Wednesdays 12:30 pm-1:20 pm, in Etherington Aud.
Fridays 11:30 am-12:20 pm, in Etherington Aud.

The full set of lecture notes will be compiled in class, any additional material will be posted on the CHEM/ENCH 212 OnQ site.

Learning goals: (i) understanding the essence of the reactivity of organic molecules and (ii) being able to relate it to kinetic studies and parameters; (iii) understanding solvent and electronic effects on reactivity. At the end of the course, students should be able to anticipate the reactivity of nearly any reactive partners.

Learning outcomes:
At the end of CHEM/ENCH 212, students will be able to……
(i) Identify reactive sites on reagents
(ii) Determine rate law expressions
(iii) Articulate the meaning of transition state parameters
(iv) Predict and justify the impact of solvent and electronic effects on reactivity
(v) Use experimental data obtained in the laboratory to study reaction kinetics, and critically analyze and communicate scientific results.

Assessment of Learning outcomes:
Tutorials will assess outcomes (i), (ii), (iii) and (iv)
Mid Term Exam will assess outcomes (i) and (iv)
Final Exam will assess outcomes (i), (ii), (iii) and (iv)
Labs will assess outcome (v)
Course Outline (with Recommended readings)

Note: Page numbers are for Atkins 10th Edition and Clayden 2nd Edition

Section 1: Chemical Reactivity: The Basics
b) Visualizing reaction mechanisms. Clayden pg. 116-124
c) Energy profiles. Clayden pg. 250-252
d) Concepts of molecular encounters. Clayden pg. 107-115

Section 2: Nucleophilic Substitution Reactions
a) Structure-reactivity relationships. Clayden pg. 332-340, pg. 344-349, pg. 351-359
b) Stereochemical outcome. Clayden pg. 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 pg. 257-262, pg. 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) How do we measure rate constants? Atkins Section 20B

Section 4: Elimination Reactions
a) General description of E1 and E2 reactions. Clayden pg. 382-387
b) Elimination vs Substitution. Clayden pg. 384-391
c) Regiochemical and stereochemical outcomes. Clayden pg. 391-399
d) The E1cb reaction. Clayden pg. 399-404

Section 5: Electrophilic Aromatic Substitution Reactions
a) General description of EAS reactions. Clayden pg. 471-478
b) Reaction of substituted benzenes. Clayden pg. 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 pg. 251-253
Supplemental Readings
These chapters are very useful as introductory and supplementary material to the CHEM 212 course. You do not need to read everything listed below! But if you feel that certain concepts presented in the lectures need 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 understanding the art of “curly arrow” drawing)*
Chapter 8: Acidity, basicity and pKas *(very good for understanding what a pKa is, and how its value changes with the structure of a molecule)*

Useful software: - free online testing and learning tools are available from the RSC website: [http://www.rsc.org/learn-chemistry/resources/mechanism-inspector/](http://www.rsc.org/learn-chemistry/resources/mechanism-inspector/)
- Several tutorials and exercises are mentioned in class as well as in the individual problem sets. Please take the time to study them: they are very useful.
- Free online reaction animations (as well as orbitals animations) are available at the following website: [http://www.chemtube3d.com/](http://www.chemtube3d.com/)
- Data processing requires Microsoft Excel

Problem sets: Practice problems and solutions will be posted on the CHEM/ENCH 212 OnQ site.
These are not marked, but are recommended, as they will help you prepare for the mid-term and final exams.

Tutorials: There are 5 tutorials throughout the semester and the dates are listed below. Please attend the time and room you selected upon enrolling. Note: Attendance at tutorials is voluntary, however, note there will be assessed group problems included in 4 out of the 5 tutorials that will make up a total of 10% of the final grade for the course. However, should a student do better in the final exam than in the tutorials, the weighting of the tutorials will be transferred onto the final exam.

Tutorial 1: Friday September 13th/Monday September 16th (2.5%)
Tutorial 2: Friday September 27th/Monday September 30th (2.5%)
Tutorial 3: Friday October 11th/Monday October 28th (No Assessment)
Tutorial 4: Friday November 8th/Monday November 11th (2.5%)
Tutorial 5: Friday November 22nd/Monday November 25th (2.5%)

Labs: All labs must be attended as scheduled
All students must attend the introductory lab (lab group assignment, lab safety, lab quiz) in week 1 (Sept. 10-12th) (~1 h)
Regular 3 h labs will be held on alternate weeks (See Schedule in onQ), in room CHE210 on the 2nd floor of Chernoff Hall.
In weeks 2-12 students will rotate between the following six experiments:
- **Experiment 1**: Photo-isomerization Kinetics of 4-Hydroxyazobenzene
- **Experiment 2**: Kinetics of Nucleophilic Substitution
- **Experiment 3**: Enzyme Kinetics – Enzyme Catalyzed Oxidation of DOPA
- **Experiment 4**: Stop-Flow Kinetics - Reaction of Fe$_{3+}$ and SCN Ions
- **Experiment 5**: Gas Viscosity – Determination of Collision Cross Section for Gases
- **Experiment 6**: Alkaline hydrolysis of Ethyl Acetate

**Course Marking Scheme:**
- Mid-term 25%, (2 h) is scheduled on **Friday October 18th, 6:30-8:30 pm**, in Chernoff Aud., Chernoff Rm 211, Chernoff Rm 213, Jeffrey Rm 101, Jeffrey Rm 127 (please contact the instructor early in case of course conflict).
- Final 40% (TBA, 3 h).
- Tutorials 10% (Sep 13/16, Sep 27/30, Nov 8/11, Nov 22/25)
- Labs: 25% (individual lab marking schemes are printed in the chem212 lab manual).

**Extra Office Hours for the Mid-term will be offered**
Timing to be announced

**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:

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<thead>
<tr>
<th>Grade</th>
<th>Numerical Course Average (Range)</th>
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<tbody>
<tr>
<td>A+</td>
<td>90-100</td>
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<tr>
<td>A</td>
<td>85-89</td>
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<tr>
<td>A-</td>
<td>80-84</td>
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<tr>
<td>B+</td>
<td>77-79</td>
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<td>B</td>
<td>73-76</td>
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<td>B-</td>
<td>70-72</td>
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<td>C+</td>
<td>67-69</td>
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<td>C</td>
<td>63-66</td>
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<tr>
<td>C-</td>
<td>60-62</td>
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<td>D+</td>
<td>57-59</td>
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<td>D</td>
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<td>F</td>
<td>49 and below</td>
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IMPORTANT:
1) The lecture material is composed of the lecture notes; they take priority over the book/online material. In the exams, you will be judged on your understanding of the lecture notes.
2) 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 a course, he/she will fail the entire course and be allocated a mark of 47% or his/her actual mark, whichever is lower. Students who do not attend all lab sessions may be assigned a grade of incomplete (IN) and be required to attend and pass the missed lab(s) the following year before the IN is cleared from their transcript.

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.”

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.

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.

**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.uslcwww/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

**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.uslcwww/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/Coordinator Name: Avena Ross
Instructor/Coordinator email address: avena.ross@queensu.ca

**Statement of the Location and 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.** Also, as indicated in Academic Regulation 8.3, students must write all final examination in all on-campus courses on the Kingston campus.