CHEM/ENCH 222 - Methods of Structural Determination
Winter Term 2018

LECTURES:  Mondays  10:30 – 11:30 am
            Wednesdays  9:30 – 10:30 am
            Fridays   8:30 – 9:30 am

            Walter Light Auditorium (Room 205)

Instructor:  Donal Macartney
            Office:  Chernoff 506
            Lab:  Chernoff 438

Instructor Contact Information:  Phone:  613-533-2617 (32617 from on-campus)
                                 E-mail:  donal@chem.queensu.ca

Office Hours:  No fixed office hours.  Drop by at any time or contact me by e-mail to make an
               appointment at a specific time.

Tutorials

Section 002  Friday 10:00 – 11:30 am  Chernoff 213
Section 003  Monday  4:00 –  5:30 pm  Chernoff 211
Section 004  Tuesday  8:30 – 10:00 am  Chernoff 213
Section 005  Tuesday  2:30 –  4:00 pm  Chernoff 213

Tutorial TAs:

Sections 002 and 004  Mai-Jan Tom  mj.tom@queensu.ca
                      613-533-6000 ext. 74776, Chernoff 539
Sections 003 and 005  Andrew Rinald  15ar49@queensu.ca
                      613-533-6000 ext. 75018, Chernoff 438

Office Hours:  No pre-set office hours; appointments by e-mail.

Tutorial Schedule

There are a total of 10 tutorial sessions, with the 5th and 10th tutorials being review sessions for
the midterm and final exams, respectively.  The remaining tutorials will be based on end-of-chapter
questions from the textbook (they will be posted on onQ in the tutorial section).  The 2nd to 4th and
7th to 9th tutorials will have also have a short quiz (highlighted in blue), comprised of 3 - 5 multiple
choice or short answer questions.  The questions will be based on the material covered in the
previous week’s tutorial and associated lecture material (details will be posted on onQ).  Note that
the 1st tutorial for section 002 is on the Friday of the first week of classes.  There are no tutorials on
the dates highlighted in yellow.
<table>
<thead>
<tr>
<th>Week</th>
<th>Tutorial Section</th>
<th>Monday 4:00 – 5:30 pm (003)</th>
<th>Tuesday 8:30 – 10:00 am (004)</th>
<th>Tuesday 2:30 – 4:00 pm (005)</th>
<th>Friday 10:00 – 11:30 am (002)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Week 1 (Jan. 8)</td>
<td>No tutorial</td>
<td>4:00 – 5:30 pm (003)</td>
<td>No tutorial</td>
<td>No tutorial</td>
<td>T1</td>
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<tr>
<td>Week 2 (Jan. 15)</td>
<td>T1</td>
<td>T1</td>
<td>T1</td>
<td>T1</td>
<td>T2 (Quiz 1)</td>
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<tr>
<td>Week 3 (Jan. 22)</td>
<td>T2 (Quiz 1)</td>
<td>T2 (Quiz 1)</td>
<td>T2 (Quiz 1)</td>
<td>T3 (Quiz 2)</td>
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<tr>
<td>Week 4 (Jan. 29)</td>
<td>T3 (Quiz 2)</td>
<td>T3 (Quiz 2)</td>
<td>T3 (Quiz 2)</td>
<td>T4 (Quiz 3)</td>
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<tr>
<td>Week 5 (Feb. 5)</td>
<td>T4 (Quiz 3)</td>
<td>T4 (Quiz 3)</td>
<td>T4 (Quiz 3)</td>
<td>T5 Midterm review</td>
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<tr>
<td>Week 6 (Feb. 12)</td>
<td>T5 Midterm review</td>
<td>T5 Midterm review</td>
<td>T5 Midterm review</td>
<td>No tutorial</td>
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<tr>
<td>Week 7 (Feb. 26)</td>
<td>No tutorial</td>
<td>No tutorial</td>
<td>No tutorial</td>
<td>T6</td>
<td></td>
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<tr>
<td>Week 8 (Mar. 5)</td>
<td>T6</td>
<td>T6</td>
<td>T6</td>
<td>T7 (Quiz 4)</td>
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<tr>
<td>Week 9 (Mar. 12)</td>
<td>T7 (Quiz 4)</td>
<td>T7 (Quiz 4)</td>
<td>T7 (Quiz 4)</td>
<td>T8 (Quiz 5)</td>
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<tr>
<td>Week 10 (Mar. 19)</td>
<td>T8 (Quiz 5)</td>
<td>T8 (Quiz 5)</td>
<td>T8 (Quiz 5)</td>
<td>T9 (Quiz 6)</td>
<td></td>
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<tr>
<td>Week 11 (Mar. 26)</td>
<td>T9 (Quiz 6)</td>
<td>T9 (Quiz 6)</td>
<td>T9 (Quiz 6)</td>
<td>Good Friday</td>
<td></td>
</tr>
<tr>
<td>Week 12 (Apr. 2)</td>
<td>T10 Final Review</td>
<td>T10 Final Review</td>
<td>T10 Final Review</td>
<td>T10 Final Review</td>
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</tbody>
</table>

**onQ site**

Students registered in the course can access the course onQ site at [https://onq.queensu.ca/d2l/home/124193](https://onq.queensu.ca/d2l/home/124193)

The site includes the lecture notes, reserve books and e-books, tutorial problems, assignments, your grades, the formula and data sheets for the midterm and exam, and other materials.

**Intended Student Learning Outcomes**

At the end of CHEM 222, students will be able to...

- Understand the basic elemental composition of organic compounds
- Define basic spectroscopic properties of organic compounds
- Discuss trends in spectroscopic properties in organic functional groups
- Analyze IR, NMR (1H, 13C and 2D), Mass and UV-vis spectra of organic compounds
- Combine all spectroscopic data given to determine the molecular structure of an unknown organic compound
- Apply Spinworks to process experimental NMR data

**Course Outline**

1st six weeks

**Chapter 1:** Molecular formulas and what can be learned from them
- Elemental analysis and calculations
- Determination of molecular mass
- Molecular formulae
- Index of hydrogen deficiency
- The rule of thirteen
Chapter 2: Infrared spectroscopy
- Molecular vibrations
- Bond properties and modes of vibration
- IR signatures of organic functional groups
- How to examine IR spectra
- General strategy in extracting structural information from IR spectra

Chapter 10: Ultraviolet spectroscopy
- Nature of electronic transition
- Organic chromophores
- Effect of conjugation
- The Beer-Lambert law
- Presentation of UV-vis spectra
- Color of organic compounds

Chapter 3: Mass spectrometry (basics)
- The mass spectrometer
- Ionization methods (EI, CI, MALDI, ESI)
- Mass analysis
- High resolution MS
- Isotope patterns

Chapter 4: Mass spectrometry (Part II)
- The Initial ionization process
- Fragmentation processes
- MS signatures of organic functional groups

2nd six weeks

Chapter 5: Nuclear magnetic resonance (Part 1)
- Nuclear spin states
- Nuclear magnetic moment
- Chemical shifts
- J-couplings
- Signal integrations

Chapter 6: Nuclear magnetic resonance (Part 2)
- $^{13}$C NMR
- Proton decoupling
- General trends in 13C chemical shifts
- Heteronuclear J-couplings
- DEPT experiments

Chapter 7: Nuclear magnetic resonance (Part 3)
- General trends in J-couplings
- Chemical and magnetic equivalency
- Strong couplings
- Spectra of diastereomers
Chapter 8: Nuclear magnetic resonance (Part 4)
- Chemical exchange processes
- $^1$H-$^{14}$N J-couplings
- The quadrupole effect
- Paramagnetic shift reagents and chiral resolving agents

Chapter 9: Nuclear magnetic resonance (Part 5)
- 2D NMR

Chapter 11: Combined Structure Problems
- Solving structures with a combination of various spectroscopic methods

Textbooks/Readings
- Required textbook: Introduction to Spectroscopy, 5th edition (Pavia, Lampman, Kriz, Vyvyan)
- Other reference books on reserve in Science Library and e-books (see list on onQ)

Grading Scheme
4 assignments: 4 x 5% 20% Approximately every 2-3 weeks
6 tutorial quizzes: 6 x 1.67% 10% See schedule above
1 midterm exam: 1 x 20% 20% Wed. Feb. 14 9:30 am – 10:30 pm (in class)
1 final exam: 1 x 50% 50% April, TBD

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

<table>
<thead>
<tr>
<th>Grade</th>
<th>Numerical Course Average (Range)</th>
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<tbody>
<tr>
<td>A+</td>
<td>90-100</td>
</tr>
<tr>
<td>A</td>
<td>85-89</td>
</tr>
<tr>
<td>A-</td>
<td>80-84</td>
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<tr>
<td>B+</td>
<td>77-79</td>
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<tr>
<td>B</td>
<td>73-76</td>
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<tr>
<td>B-</td>
<td>70-72</td>
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<tr>
<td>C+</td>
<td>67-69</td>
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<tr>
<td>C</td>
<td>63-66</td>
</tr>
<tr>
<td>C-</td>
<td>60-62</td>
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<tr>
<td>D+</td>
<td>57-59</td>
</tr>
<tr>
<td>D</td>
<td>53-56</td>
</tr>
<tr>
<td>D-</td>
<td>50-52</td>
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<tr>
<td>F</td>
<td>49 and below</td>
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</tbody>
</table>
Late Policy
If you require additional time to complete an assignment please contact me as soon as possible. See below for the Chemistry Department policy on missed quizzes, tests, midterms, presentations, and assignments.

Department of Chemistry Policy on Missed Quizzes, Tests, Midterms, Presentations, and Assignments
The Chemistry Department requires that students submit a ‘declaration of extenuating circumstances’ form before being considered for accommodation. The form, and related information, is available at http://www.chem.queensu.ca/undergraduate/undergraduate-resources/missed-exam-policy. Note that this departmental policy does NOT apply to final exams.

Tutorial Information
During each 1.5-hour tutorial section, the TA will work through the end-of-chapter questions assigned for each chapter. The TA will also hold a Q&A session about the concepts learned in the previous week. In six of the ten tutorials (see schedule above) there will be a short quiz based on the previous week’s lecture and tutorial material. The TA will also discuss the previous assignment in the week it is returned to students.

Calculator Policy
Calculators are not permitted (or needed) for the tutorial quizzes, nor the midterm and final examinations.

Academic Integrity
Academic Integrity is constituted by the five core fundamental values of honesty, trust, fairness, respect and responsibility (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 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 http://www.queensu.ca/artsci/academics/undergraduate/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
All materials associated with this course are copyrighted. This includes in-class handouts, E-mailed information, and all documents and information provided on the course onQ site. These course materials are for the sole use of students registered in the course. These materials shall not be distributed or disseminated to anyone other than students registered in this course. Failure to abide by these conditions is a breach of copyright, and may also constitute a breach of academic integrity under the University Senate’s Academic Integrity policy statement.
**Accessibility Statement**
Queen’s is committed to an inclusive campus community with accessible goods, services, and facilities that respect the dignity and independence of persons with disabilities. Course materials are available in an accessible format or with appropriate communication supports upon request.

Please contact Meredith Richards in the Department of Chemistry in one of the following ways:
- Email: ugadm@chem.queensu.ca
- Phone: 613-533-6000 extension 75518
- In person: Chernoff 200

**Accommodations Statement**
Queen’s University is committed to achieving full accessibility for persons 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. If you are a student with a disability and think you may need accommodations, you are strongly encouraged to contact Student Wellness Services (SWS) and register as early as possible. For more information, including important deadlines, please visit the Student Wellness website at: [http://www.queensu.ca/studentwellness/accessibility-services/](http://www.queensu.ca/studentwellness/accessibility-services/)

**Academic Considerations for Students in Extenuating Circumstances**
The Senate Policy on Academic Consideration for Students in Extenuating Circumstances ([http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslcwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf](http://www.queensu.ca/secretariat/sites/webpublish.queensu.ca.uslcwww/files/files/policies/senateandtrustees/Academic%20Considerations%20for%20Extenuating%20Circumstances%20Policy%20Final.pdf)) was approved in April 2017. Queen’s University is committed to providing academic consideration to students experiencing extenuating circumstances that are beyond their control and which have a direct and substantial impact on their ability to meet essential academic requirements. The Faculty of Arts and Science has developed a protocol to provide a consistent and equitable approach in dealing with requests for academic consideration for students facing extenuating circumstances, which can be found at: [http://www.queensu.ca/artsci/accommodations](http://www.queensu.ca/artsci/accommodations)

**Statement of the Location and Timing of Final Examinations**
As noted in Academic Regulation 8.2.1, “the final examination in any class offered in a term or session (including Summer Term) must be written on the campus on which it was taken, at the end of the appropriate term or session at the time scheduled by the Examinations Office.” The exam period is listed in the key dates prior to the start of the academic year in the Faculty of Arts and Science Academic Calendar and on the Office of the University Registrar’s webpage. A detailed exam schedule for the Fall Term is posted before the Thanksgiving holiday; for the Winter Term it is posted the Friday before Reading Week, and for the Summer Term the window of dates is noted on the Arts and Science Online syllabus prior to the start of the course. 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.