

CHEM/ENCH 222 - Methods of Structural Determination

Winter Term 2023

LECTURES: Monday 1:30 PM – 2:30 PM (STIRLING AUD)
Wednesday 12:30 PM – 1:30 PM (STIRLING AUD)
Friday 11:30 AM – 12:30 PM (STIRLING AUD)

Instructor: Prof. Gang Wu

Instructor Contact Information: E-mail: wugang@queensu.ca

Virtual Office Hours: Tuesdays at 10-11 AM (MS Teams meetings)

Tutorials

Section 002 Thursday 2:30 PM – 4:00 PM (MCLAUGHLIN RM306)
Section 003 Thursday 8:30 AM – 10:00 AM (BOTTER RM B139)
Section 004 Thursday 4:00 PM – 5:30 PM (NICOL RM321)
Section 005 Thursday 2:30 PM – 4:00 PM (STIRLING RM414)

Tutorial TAs:

Jennifer Kolwich Sections 002 and 004
jlk8@queensu.ca

Lukas Bauder Section 003
bmqv@queensu.ca

Angus Sullivan Section 005
ais4@queensu.ca

Schedules for Tutorials and Quizzes

Tutorials: There will be a total of 10 tutorial sessions. The tutorials will be based on end-of-chapter (EOC) questions from the textbook (the questions will be posted on onQ in “Tutorial Questions” section). TAs will solve these problems during tutorials.

Quizzes: A total of 6 quizzes are scheduled as shown below. Each quiz consists of 5 randomized multiple-choice questions based on the material learned in the previous one or two weeks. The quiz will be taken through onQ during the Thursdays as indicated in the following table. You can start the quiz at any time during the specified day (from 9 AM to 11:59 PM). Once you start the quiz, you will have 15 min to finish it.

Week	Tutorial	Quiz
1 (Jan. 9-13, 2023)	No tutorial	No quiz
2 (Jan. 16-20)	Tutorial 1	No quiz
3 (Jan. 23-27)	Tutorial 2	Quiz 1 (Jan.26, 2023)
4 (Jan. 30-Feb.3)	Tutorial 3	Quiz 2 (Feb.2, 2023)
5 (Feb. 6-10)	Tutorial 4	Quiz 3 (Feb.9, 2023)
6 (Feb. 13-17)	No tutorial	No quiz
7 Reading Week (Feb.21-24)	No tutorial	No quiz
8 (Feb. 27-Mar.3)	No tutorial	No quiz
9 (Mar. 6-10)	Tutorial 5	Quiz 4 (Mar.9, 2023)
10 (Mar. 13-17)	Tutorial 6	Quiz 5 (Mar.16, 2023)
11 (Mar. 20-24)	Tutorial 7	Quiz 6 (Mar. 23, 2023)
12 (Mar. 27-31)	Tutorial 8	No quiz
13 (Apr. 3-7)	Tutorial 9	No quiz

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 , ^{13}C 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 software to process experimental NMR data

onQ site

Students registered in the course can access the course onQ site at

<https://onq.queensu.ca/d2l/home/692050>

The site includes the lecture notes/videos, reserve books and e-books, tutorial problems and quizzes, assignments, your grades, the formula and data sheets for the midterm and final exam, old exams with solutions, and other materials.

Textbook, Reserve Books, E-books

The textbook for the course is "Introduction to Spectroscopy", 5th edition by Pavia, Lampman, Kriz, and Vyvyan (available in the Campus Bookstore). This book is also available on Amazon (new and used).

Some useful books in Douglas science library at Queen's are listed below.

QD272.S6 S74 2002	Organic structures from spectra, 3 rd ed.	Field, Sternhell, Kalman
QD272.S6 T33 2007	Organic spectroscopic structure	Taber

	determination: a problem-based learning approach	
QD272.S6 O74 2011	Organic structural spectroscopy, 2 nd ed	Lambert et al.
QD272.S6 W54 1995	Spectroscopic methods in organic chemistry	Williams, Fleming
QD272.S6 S55 2005	Spectroscopic identification of organic compounds, 7 th ed.	Silverstein, Webster, Kiernle
QD272.S6 Y33 2005	Organic spectroscopy	Yadav

E-books

Structure determination of organic compounds – tables of spectra data

<http://link.springer.com/book/10.1007%2F978-3-540-93810-1>

Organic Structure Determination Using 2-D NMR Spectroscopy - A Problem-Based Approach (2nd Edition)

http://app.knovel.com/web/toc.v/cid:kpOSDUDNM1/viewerType:toc/root_slug:organic-structure-determination

Organic Spectroscopy – Yadav

<http://link.springer.com/book/10.1007%2F978-1-4020-2575-4>

Course Outline (Textbook chapters)

First Half (Weeks 1-6)

- 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 (Part 1 and Part 2)
- 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 3: Mass spectrometry (Part 1)

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

- Chapter 4: Mass spectrometry (Part 2)
- The Initial ionization process
 - Fragmentation processes
 - MS signatures of organic functional groups

Second Half (Weeks 8-13)

- 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 ^{13}C 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
 - ^1H - ^{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

Grading Scheme

4 Assignments:	4 x 10%	40%	Approximately every 2 weeks
6 Quizzes:	5 x 2%	10%	See quiz schedule shown above
	(best 5 out of 6 quizzes)		
1 Midterm exam:	1 x 10%	10%	11:30 AM - 12:30 PM, Friday, Feb. 17, 2023
1 Final Exam:	1 x 40%	40%	A regular 3-hour in-person exam (date 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

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

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.

Calculator Policy

Calculators are not needed, nor allowed, during the midterm or final exams, or the tutorial quizzes. You are welcome to use calculators for the assignments or tutorial problems.

Academic Integrity

Academic Integrity is constituted by the six core fundamental values of 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 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 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/senateandtruste/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, not to exceed three months. Students receiving academic consideration must meet all essential requirements of a course. The Senate Policy on Academic Consideration for Students in Extenuating Circumstances was approved at Senate in April, 2017 (see <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/Coordinator Name: Prof. Gang Wu

Instructor/Coordinator email address: wugang@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.

Turnitin Statement

This course makes use of Turnitin, a third-party application that helps maintain standards of excellence in academic integrity. Normally, students will be required to submit their course assignments to through onQ to Turnitin. In doing so, students' work will be included as source documents in the Turnitin reference database, where they will be used solely for the purpose of detecting plagiarism.

Turnitin is a suite of tools that provide instructors with information about the authenticity of submitted work and facilitates the process of grading. Turnitin compares submitted files against its extensive database of content, and produces a similarity report and a similarity score for each assignment. A similarity score is the percentage of a document that is similar to content held within the database. Turnitin does not determine if an instance of plagiarism has occurred. Instead, it gives instructors the information they need to determine the authenticity of work as a part of a larger process.

Please read [Turnitin's Privacy Pledge, Privacy Policy, and Terms of Service](#), which governs users' relationship with Turnitin. Also, please note that Turnitin uses cookies and other tracking technologies; however, in its service contract with Queen's Turnitin has agreed that neither Turnitin nor its third-party partners will use data collected through cookies or other tracking technologies for marketing or advertising purposes. For further information about how you can exercise control over cookies, see [Turnitin's Privacy Policy](#).

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