

CHEM/ENCH 322 – Molecules and Spectroscopy

Winter Term 2022

Lectures: Tuesday — 8:30-9:30 am
 Wednesday — 10:30-11:30 am
 Friday — 9:30-10:30 am

(All lecture notes/videos will be posted on Q and can be viewed [asynchronously](#))

Instructor: Prof. Gang Wu

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

Virtual Office Hours: Wednesday at 10-11 am (Teams meetings)

Online tutorials (synchronous)

Tutorial section 002 Mondays 11:30 am – 12:30 pm
Tutorial section 003 Wednesday 11:30 am – 12:30 pm
Tutorial section 004 Wednesday 8:30 – 9:30 pm

Tutorial TA: Carolyn Kimball (Email: cmk8@queensu.ca) sections 002 and 003
 Sangeeth Das Kallullathil (Email: sdk4@queensu.ca) section 004

Course Schedule

The tutorial questions will be posted on the course onQ site under “Tutorial Problems”.

Week	Topic	Tutorial	Assignment
1 (Jan. 10-14, 2022)	Atomic Spectroscopy (I)	No tutorial	Assignment 1 due on 10 am Jan. 31, 2022 (Monday)
2 (Jan. 18-22)	Atomic Spectroscopy (II)	Tutorial 1	
3 (Jan. 25-29)	Molecular Spectroscopy (I)	Tutorial 2	
4 (Feb. 1-5)	Molecular Spectroscopy (II)	Tutorial 3	Assignment 2 due on 10 am Feb.18, 2022 (Friday)
5 (Feb. 8-12)	Molecular Spectroscopy (III)	Tutorial 4	
6 (Feb. 14-18)	Review and Midterm	No tutorial	
7 Reading Week (Feb.21-25)			
8 (Feb.28-Mar.4)	NMR Spectroscopy (I)	No tutorial	Assignment 3 due on 10 am Mar.21, 2022 (Monday)
9 (Mar. 7-11)	NMR Spectroscopy (II)	Tutorial 5	
10 (Mar. 14-18)	NMR Spectroscopy (III)	Tutorial 6	
11 (Mar. 21-25)	NMR Spectroscopy (VI)	Tutorial 7	Assignment 4 due on 10 am April 8, 2022
12 (Mar. 28-Apr.1)	NMR Spectroscopy (V)	Tutorial 8	

13 (Apr. 4-8)	Review	Tutorial 9	(Friday)
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Intended Student Learning Outcomes

At the end of CHEM 322, students will be able to...

- Understand the basic process of spectral analysis
- Understand atomic spectra including fine structures from hyperfine interactions
- Analyze rotational spectra of diatomic molecules
- Analyze ro-vibrational spectra of diatomic molecules
- Recognize patterns in electronic spectra of polyatomic molecules
- Understand the basics of NMR spectroscopy

CHEM322 course onQ site

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

<https://onq.queensu.ca/d2l/home/603405>

The site includes the lecture notes/videos, tutorial problems, assignments, midterm test, final exam, grades, the formula and data sheets for the midterm and final exam, and other materials.

Textbooks

Recommended textbooks:

- (1) T. P. Softley, "Atomic Spectra", Oxford Chemistry Primers, #19
- (2) John M. Brown, "Molecular Spectroscopy", Oxford Chemistry Primers, #55
- (3) Peter J. Hore, "Nuclear Magnetic Resonance", Oxford Chemistry Primers, #32

NOTE: This course is primarily based on lecture notes, because I cannot find a single textbook available to date that would cover all the topics taught in this course. The above-listed texts are only recommended to be used as references. Since these books have been used in the past, you may be able to find some second-hand copies.

Course Outline

First Half (Weeks 1-6)

Atomic Spectroscopy

- Hydrogen spectrum
- Boltzmann law
- Many-electron atoms
- Spin-orbit coupling and term symbols

- Hyperfine interaction

Molecular Spectroscopy

- Rotational Spectroscopy (the rotational Hamiltonian, Rotational wavefunctions and symmetry, Centrifugal distortion, Structural determination from rotational spectra, The Stark effect)
- Vibrational Spectroscopy (Harmonic oscillator, Eigenvalues and eigenfunctions, The anharmonic oscillator, Vibration-rotation spectra)
- Raman Spectroscopy (Raman scattering, Rotational Raman spectra, Raman spectra of diatomic molecules, Nuclear spin statistical weights, Rotational Raman spectra of symmetric and asymmetric rotors, Vibrational Raman spectra)
- Electronic Spectroscopy (Molecular orbitals and electronic states of molecules, Electronic selection rules, Potential energy curves, Vibrational and rotational fine structures)

Second Half (Weeks 8-13)

Nuclear Magnetic Resonance

- Nuclear spins, Zeeman interaction
- Vector model and Bloch equation
- Free induction decay
- Chemical shifts and spin-spin couplings
- Spin relaxation
- 2D NMR
- Applications in structural biology (protein NMR)
- Applications in medicine (MRI)

Grading Scheme

4 Assignments:	4 x 10%	40%	Approximately every 3 weeks
1 Midterm exam:	1 x 25%	25%	7:00 – 9:00 pm, Thursday, Feb. 17, 2022
1 Final exam:	1 x 35%	35%	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)
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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/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, 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.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: 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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