DEPARTMENT OF CHEMISTRY UNIVERSITY OF TORONTO

CHM1455HS LEC0101 NMR Spectroscopy Course Outline - Winter 2024

Class Location & Time Fri, 11:00 AM - 01:00 PM MN2210

InstructorAmy JenneOffice LocationCCT4122

Office Hours Friday 9:30-10:30, or virtual by appointment

E-mail Address amy.jenne@utoronto.ca
Course Web Site https://q.utoronto.ca

Kindness Statement

I would like each of us to approach this semester and our interactions with kindness at the forefront. I will be treating you with kindness and respect and please ask that you do the same. Remember we are all here to learn together, support one another, and we do not know what other people are going through in their lives. There is enough negativity in the world, let's make this space a positive one. I am thrilled that you are joining this space and incredibly excited for the upcoming semester!

Acknowledgement of Traditional Lands

We wish to acknowledge this land on which the University of Toronto operates. For thousands of years it has been the traditional land of the Huron-Wendat, the Seneca, and the Mississaugas of the Credit. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.

If you are interested in learning more about the land you are occupying, please see: https://native-land.ca/.

Course Description

Fundamentals of Nuclear Magnetic Resonance (NMR) spectroscopy including classical and quantum descriptions, NMR parameters and relaxation times, product operators, multi-dimensional NMR, and solid-state techniques.

Course Learning Outcomes

On successful completion of the course, you will be able to:

- 1. Understand fundamental concepts in NMR spectroscopy.
- 2. Describe spin dynamics using both classical and quantum descriptions.
- 3. Gain experience in data processing and analysis using software packages.
- 4. Understand theoretical and practical aspects of multidimensional NMR.
- 5. Describe fundamentals mechanisms of spin relaxation and molecular dynamics.
- 6. Appreciate and describe modern methods and applications of NMR spectroscopy.

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- 7. Create a thoughtful, seminar-style, oral presentation on current trends in a particular area of NMR science research and development.
- 8. Write a major critical review paper on a topic of current research in NMR research and development.

Textbooks (recommended):

Keeler, J. (2010). Understanding NMR Spectroscopy (2nd edition). Wiley.

Assessment and Grading

Type	Description	Due Date	Weight
Assignment	Choice 1, Due at 11:59 pm	2024-02-02	10%
Assignment	Choice 2, Due at 11:59 pm	2024-03-01	20%
Presentation	Seminar Presentation	Ongoing	30%
Assignment	Term Paper, Due at 11:59 pm	2024-04-08	40%

^{*}Note that only the grades for Choice assignment 1 will be returned by the drop date for the course.

Other Course Content Information

Lecture Schedule

The following table provides a tentative schedule of the topics to be covered during the various lecture sessions throughout the term. While you are responsible for the topics covered, I understand that events can occur which impact participation. In such an event, you are encouraged to read through the materials posted on Quercus, read the related chapters of the textbook, get in touch with a classmate, and/or visit me during Office Hours to ensure that you are prepared for any assignments or presentations related to the topic in question. Additionally, you'll note in the schedule, that this course is cross-listed with an undergraduate course. Your course structure is slightly different then undergraduate students, but the breakdown below is specific to CHM1455.

Date	Topic	Date	Topic
Jan 12	Introduction to NMR Parameters	Jan 19	Introduction to NMR Parameters
Jan 26	Vector Description of NMR	Feb 2	NMR Data and Fourier Transform
Feb 9	Product Operator Formalism	Feb 16	2D NMR
Feb 23	Reading Week	Mar 1	Relaxation and Dynamics
Mar 8	Fluorine NMR and Advanced Topics in NMR	Mar 15	Advanced Topics in NMR
Mar 22	Undergraduate Paper Presentations	Mar 29	Good Friday – No Class
Apr 5	Graduate Student Seminars	Monday Apr 8	Graduate Student Seminars

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Assignment Breakdown

Below all the course assignments are introduced, so you know what to expect. This year, we are trying something different in this course. 70% of the assignments everyone will participate in, but the other 30% will be 'buffet style' which means that you may choose the forms of assessment which work best for you. The options for these are below, but if you have something else you are interested in pursuing, let me know and we can discuss. Full details for all assignments as well as templates will be posted to Quercus.

Quizzes

Each week, after lecture, a quiz will open on Quercus based on content learned from lecture. These quizzes are optional if you would like extra practice. You will have until the start of the next lecture to complete the quiz.

Seminar Presentations

Students will present a twenty (25) minute seminar on an NMR topic. You're welcome to present on a topic of your own research but must be focused on the methods and applications of NMR. Please leave time (5 minutes) at the end for questions as the undergraduate students are awarded marks for class participation. The audience should walk away with a clear message of what, why, and how. The audience should also gain an appreciation of the unique or novel aspects of the topic, as well as its potential impact on our lives. Presentations are scheduled for Friday April 5th or Monday April 8th; presentation order will be assigned randomly. Topics must be approved via email by Friday January 26th by 5:00 pm.

Term Paper

The topic selected for your term paper should be researched and written independently in the form of a critical review. Your review should begin with a thoughtful overview of the field and introduction to the fundamental science and key concepts as required for your reader to gain an appreciation of the topic. A good review article will allow a non-expert to the field to gain a good understanding of the key scientific concepts and operating principles of all methods (including specifics required to understand specific NMR experiments) discussed and all instrumentation used in all analyses described in your paper.

Topic selection must be approved, by emailing me, by Friday January 26th at 5:00 pm. Additionally, you may choose to submit a draft for instructor feedback. This is optional and not for marks, but may be useful if you would like feedback prior to full paper submission. The deadline for submission to receive feedback is Monday February 26th at 5:00 pm.

Choice Assignments

This is where you as a student, get to control aspects of your learning! Below there are two sections of assignments. You must choose one (1) option from category A, and one (1) option from category B. Full Learning objectives and expectations will be posted to Quercus. Total you will be completing two (2) assignments, but you get to choose! These assignments will be worth 30% of your grade, but will be broken down into 20% and 10%. The assignment which you score the best on will be weighted as the 20% assignment at the end of term. Thus, even though "Choice 2" in the mark breakdown above is listed as 20%, if you do better on one of the other assignments, it

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will become worth 20%. You may submit either assignment on each of the deadlines and in any combination so long as you submit one from each category.

Category A: Course Concept Applications (Choose 1)	Category B: Real-World NMR Application (Choose 1)		
 Solve a case study. Design an experiment. Create 3 exam questions with solutions. Propose something - must be preapproved by the instructor. 	 Write a blog post on a course topic (for a nonexpert). Create a(n) infographic/podcast/TikTok on a course topic (for a non-expert). Note: you will choose one of these, not all three. Complete a profile on a marginalized NMR scientist. Propose something - must be preapproved by the instructor. 		
Examples: Case Study & Podcast OR Diverse Chemist & Expe	riment Design OR Exam Questions & TikTok etc		

Due: Feb 2, Mar 1

Procedures and Rules

Missed Term Work and Tests, Late Penalties and Absence Declarations

Penalties for all term work missed or otherwise submitted late is as described in the text that follows unless valid and documented reasons exist for special consideration. Students may submit a petition for special consideration within one week of the due date of the missed item of term work or date of the missed test.

The ACORN absence declaration system may be used once per term, to declare an absence of up to seven consecutive calendar days (including days both before and after the date of submission), without requiring medical or other documentation. Provide the Course Instructor with a confirmation of this declaration (e.g. a screenshot) in your petition for special consideration, which contains your name, student number, absence dates, and confirmation number. For more information on the ACORN absence declaration process, and to access the form, see here.

In all other cases (beyond the above-described once-per-term declaration), documentation is required. In all cases, petitions for special consideration should be based on illness or other extenuating circumstances, which are beyond one's reasonable control. Note that reasons such as vacations, family events, wedding attendance, lack of preparation, technology failure, extracurricular commitments, and academic work in other courses are not considered to constitute extenuating circumstances beyond a student's reasonable control. Absences for reasons of illness should be documented using the <u>U of T Verification of Student Illness or Injury form</u>; please complete this form, have it signed by the appropriate professional (e.g. a medical doctor), and send a copy to the course instructor. If not for reasons of illness, your petition for special consideration must contain supporting documentation, which can include a <u>U of T Verification of Extenuating Circumstances</u> form, automobile collision or police reports, a death certificate, and supporting documentation from employers, lawyers and other professional persons. Supporting documents can be submitted electronically as an attachment in your e-mail to the Course Instructor. These attachments can include screenshots, photographs, and/or scans of physical documents. Please

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ensure the electronic documents are legible and also ensure that you retain the original copies of all documents submitted in case you are asked to present them later. The supporting documentation included in your petition must specify the exact period that you were unable to complete your term work or term test for it to be considered. The Course Instructor will inform the student by e-mail (as per the Communications Policy herein) whether special consideration is granted following due diligence on the documentation provided. Note that false statements and/or documentation will be treated as academic offences and handled accordingly.

The penalty for late submission of term work (e.g. assignments, quizzes, etc.) is a 10% deduction in the final mark per day that the work is late. A late penalty may be waived provided that a petition for special consideration is made and granted as described above.

If a student is absent for their presentation, a mark of **zero** (0%) will be assigned as their presentation mark unless special consideration is granted, as specified above. The mark value of the presentation will be re-assigned to term paper (i.e., the term test will be worth an additional 30% of the total mark for the course, e.g., 70% from 40%), provided that special consideration is granted.

Re-evaluation Requests

Requests for re-evaluation of an article of term work (e.g. assignment, quizzes, etc.) must be made in writing within **1 month** of the return of the article of term work and include a brief explanation as to why the request is being made. Term work submissions can be written in pencil; however, re-marking of term work written in pencil is not permitted. Similarly, articles of term work on which correction media has been used will be exempt from re-evaluation. Re-evaluation requests must be made to the same person that did the initial grading of the article of term work. Note that the final mark assigned to a re-evaluated article of term-work may go up or down based on the outcomes of re-evaluation (in whole or in part, at the discretion of the marker). As a UofT student, have the right to appeal a mark beyond the Course Instructor only if the term work in question is worth at least 20% of the course mark.

Communications Policy

Students are welcome and encouraged to meet with me during the posted office hour. Office hours will be in-person. Additionally, visits outside of the regularly scheduled office hour(s) (in-person or virtually) can be made by appointment. Feel free to also email me if you have any concerns. I will endeavour to respond to e-mail within two workdays at the latest.

Privacy and Use of Course Materials/Copyright

All course materials belong to the Course Instructor, the University, and/or other sources (depending on the specific facts of each situation) and are protected by copyright. In this course, you are permitted to download materials for your own academic use, but you should not copy, share, or use them for any other purpose without the explicit permission of the Course Instructor. In the event of a mandated switch to remote course delivery, this course, including your participation, will be recorded on video and will be available to students in the course for viewing remotely and after each session. Course videos and materials belong to your instructor, the University, and/or other sources depending on the specific facts of each situation, and are protected by copyright. In this course, you are permitted to download session videos and materials for your

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own academic use, but you should not copy, share, or use them for any other purpose without the explicit permission of the instructor. For questions about recording and use of videos in which you appear please contact your instructor.

Academic Integrity

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The <u>University of Toronto's Code of Behaviour on Academic Matters</u> outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see www.academicintegrity.utoronto.ca/).

Academic Rights

You, as a student, have the right to:

- Receive a syllabus by the first day of class.
- Rely upon a syllabus once a course is started. An instructor may only change marks' assignments by following the University Assessment and Grading Practices Policy provision 1.3.
- Refuse to use the University's plagiarism detection tool (you must be offered an alternative form of submission).
- Have access to your Instructor for consultation during a course or follow up with the Department Chair if the Instructor is unavailable.
- Receive at least one significant mark (15% for H courses, 25% for Y courses) before the last day you can drop a course for H courses, and the last day of classes in the first week of January for Y courses taught in the Fall/Winter terms.
- Submit handwritten essays so long as they are neatly written.
- Have no assignment worth 100% of your final grade.
- Not have a term test worth 25% or more in the last two weeks of class.
- Retain intellectual property rights to your research.
- Receive all your assignments once graded.
- Privacy of your final grades.
- Arrange for representation from Downtown Legal Services (DLS), and/or other forms of support if you are charged with an academic offence.

Inclusivity Statement

You belong <u>here</u>. The University of Toronto commits to all students, faculty, and staff that you can learn, work, and create in a welcoming, respectful, and inclusive environment. In this class, we embrace the broadest range of people and encourage their diverse perspectives. This team

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environment is how we will innovate and improve our collective academic success. You can read the evidence for this approach here.

We expect each of us to take responsibility for the impact that our language, actions and interactions have on others. You have rights under the Ontario Human Rights Code. If you experience or witness any form of harassment or discrimination, including but not limited to, acts of racism, sexism, Islamophobia, anti- Semitism, homophobia, transphobia, ableism and ageism, please tell someone so that we can intervene. You can talk to anyone you feel comfortable approaching, including your me, members of the CPS Equity, Diversity and Inclusivity Committee, or any staff member at our Equity, Diversity & Inclusion Office.

You are not alone. Working together, we can all achieve our full potential.

Course Code of Conduct and Expectations

Each member of this course is expected to maintain:

- A professional and respectful attitude during all course activities.
- A personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
- Backup copies of all work. Electronic backups should be maintained (ideally in real time) to circumvent technology failures that would otherwise prevent completion of assignments on time. Note that all UofT students are provided with 1 TB of cloud-based storage on the Office365 OneDrive platform (hosted by Microsoft Canada). All students are encouraged to maintain a live backup copy of their work using this secure, cloud-based platform.
- A collection of class notes recorded independently based on concepts covered in lectures and labs (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation).
- Familiarity with the University's policy on Academic Integrity (see: the section entitled Academic Integrity, above, and the <u>Code of Behaviour on Academic Matters</u>).
- Familiarity with the <u>University policy on Sexual Violence and Sexual Harassment</u>. Note that sexual violence is any sexual act or act targeting a person's sexuality, gender identity or gender expression, whether the act is physical or psychological in nature, that is committed, threatened or attempted against a person without the person's consent. All members of the University community should have the ability to study, work, and live in an environment free from sexual violence and sexual harassment.

Equity Statement

The University of Toronto is committed to equity and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. I will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course, and I wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our Equity Offices.

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Accommodations for Learning Needs

The University of Toronto Mississauga supports accommodations for students with diverse learning needs, which may be associated with mental health conditions, learning disabilities, autism spectrum, ADHD, mobility impairments, functional/fine motor impairments, concussion or head injury, blindness and low vision, chronic health conditions, addictions, deafness and hearing loss, communication disorders and/or temporary disabilities, such as fractures and severe sprains, or recovery from an operation.

If you have a learning need requiring an accommodation, we recommend that students register as soon as possible with <u>Accessibility Services</u>.

Phone: 905-569-4699

Email: access.utm@utoronto.ca

Accommodations for Religious Observations

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, lab session, or lecture. Students must inform the instructor before the session/assignment date to arrange accommodations.

Additional Services and Support

The following are some important links to help you with academic and/or technical service and support:

- School of Graduate Studies' <u>Policies and Guidelines</u>.
- Full library service and resources on conducting online research through University of Toronto Libraries <u>University Libraries Research</u>.
- Resources on academic support from the Academic Success Centre.
- Learner support at the Writing Centre.
- Information for Technical Support/Ouercus Support.

Mental Health

As a university student, you may experience a range of health and/or mental health challenges that could result in significant barriers to achieving your personal and academic goals. Please note, the University of Toronto (St. George and Mississauga campuses) offer a wide range of free and confidential services that could assist you during these times.

Other resources include:

- Accessibility Services
- Health & Wellness (St. George)
- Health & Counselling Centre (UTM)
- My Student Support Program (MySSP)
- Good2Talk Student Helpline
- Navi
- Toronto Distress Centre (416-408-4357)

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If you find yourself feeling distressed and in need of more immediate support resources, consider reaching out to the counsellors at <u>My Student Support Program (MySSP)</u> or visiting the <u>Feeling Distressed webpage</u>.

You are not alone, and it's okay to need help, please ask for it.

Additional Dates of Significance

January 8, 2024: Classes begin for S and Y courses.

February 20, 2024: Last day to drop an S course without academic penalty.

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