DALHOUSIE UNIVERSITY

Department of Chemistry
Organic Structure Determination
Chemistry 4402/5402
Winter 2024

Dalhousie University acknowledges that we are in Mi'kma'ki, the ancestral and unceded territory of the Mi'kmaq People and pays respect to the Indigenous knowledges held by the Mi'kmaq People, and to the wisdom of their Elders past and present. The Mi'kmaq People signed Peace and Friendship Treaties with the Crown, and section 35 of the Constitution Act, 1982 recognizes and affirms Aboriginal and Treaty rights. We are all Treaty people.

Dalhousie University also acknowledges the histories, contributions, and legacies of African Nova Scotians, who have been here for over 400 years.

Instructor: Professor Norm Schepp, nschepp@dal.ca, Room 411
Lectures: Tuesday & Thursday, 10:05 to 11:25 am, LSC C332

Course Description (from the Calendar):

"Nuclear magnetic resonance spectroscopy and mass spectrometry are emphasized in solving structural problems. Topics include 2D NMR, correlation of structure with chemical shifts and coupling constants, operation of NMR spectrometers, NMR relaxation, analysis of spectral patterns, the vector model of 1D and 2D experiments and ionization methods in mass spectrometry."

Course Prerequisites

CHEM 3404 is the prerequisite for CHEM 4402.
Chem 4402 and 5402 are crosslisted. Credit cannot be obtained for both 4402 and 5402.

Course Objectives/Learning Outcomes

- ability to interpret spectroscopic data for compound identification.

Course Materials

- **Lecture** notes (PowerPoint slides) will be available on Brightspace.
- **Problem solving** lectures will be available during the term as given in the schedule. These lectures will focus on showing and solving sample NMR problems, as well as describing some techniques for solving NMR problems.

DALHOUSIE UNIVERSITY

- **There is no textbook for this class.**
- **Problem sets** and answers will be available on the Brightspace class website. No marks will be awarded for completing the posted problem sets, but working on the problems – as opposed to just looking at the answers – will be a good way to find out if you have grasped the material and will be excellent training for the midterms and the final examination.

Course Assessment

Online quizzes	3 or 4 Online (Brightspace) quizzes; dates TBD	20%
Midterm 1	Feb 13, in-class	10 %
Midterm 2	March 12, in-class	15 %
Take home Test	March 21 out – March 26 in (in-class)	20 %
Final Exam	3 hr, in-person, during exam schedule	35 %

Conversion of numerical grades to Final Letter Grades follows the Dalhousie Common Grade Scale

For Chem 4402:

A+ (90-100)	**B+** (77-79)	**C+** (65-69)	**D**	(50-54)
A (85-89)	**B** (73-76)	**C** (60-64)	**F**	(<50)
A- (80-84)	**B-** (70-72)	**C-** (55-59)		

For Chem 5402:

A+ (90-100)	**A-** (80-84)	**B** (73-76)	**F**	(<70)
A (85-89)	**B+** (77-79)	**B-** (70-72)		

Course Policies

Office hours: Room 411, Tues and Thurs, 1:30 to 2:30 (subject to change). You can also send me an email to arrange an appointment for an in-person meeting in Room 411 when you have questions. You can also drop-in to Room 411 at any time and see if I am available.

Email: It is your responsibility to read your Dalhousie email, as class notifications may be sent by email.

Course Policies on Missed or Late Academic Requirement

If you are ill or otherwise experiencing a personal emergency at the time of a midterm test, e-mail me when convenient to inform me of the situation, and fill out a Student Declaration of Absence form at an appropriate time (within two (2) days of the date of the test.) Many circumstances can count as personal emergencies, and I am happy to help you to

the best of my ability in accommodating unexpected life circumstances that may take priority over this course for you.

Make-ups are not offered for midterm exams or on-line quizzes. In case any of these evaluation elements are missed due to illness or a prearranged situation, the weighting of the final exam will change to make up the missing marks.

The Take Home test must be submitted on time and will not be accepted after the due date. No make-up Take Home test will be offered.

If you are ill for the final exam, notify me prior to the start of the final exam. A make-up final exam will be offered.

Course Policies related to Academic Integrity

You are required to complete quizzes and the Take Home test ON YOUR OWN, without any outside assistance of any kind, including assistance from other classmates.

Course Content

This class will teach the use of spectroscopic methods to determine the structures of organic compounds. By far one of the most important technique used for the determination of organic structures is NMR. This will mean that 95% of the content will be NMR spectroscopy, of which roughly 90% will be ^{1}H and ^{13}C NMR.
The class will not dwell on theoretical aspects, although in places limited appreciation of some very basic physics will be expected. Some useful information about mass spectrometry (MS) and infrared (IR) spectroscopy may be presented if time permits. Students are responsible for all of the material covered in the lectures. There is no laboratory component to this class.

Topics to be covered include (order subject to change):

- Basic theory of NMR spectroscopy
- NMR Chemical shifts and coupling constants with a heavy emphasis on ^{1}H and ^{13}C NMR (some ^{19}F and ^{31}P NMR)
- Issues of NMR spectral complexity: first and second order spectra
- 1D ^{13}C NMR spectra as well as DEPT
- 2D NMR spectra (COSY, HETCOR, TOCSY, HSQC, HMQC, HMBC)
- NMR Relaxation phenomena
- NOE: its measurement and exploitation
- Dynamic NMR
- Overview of the useful aspects of IR (If time permits)
- Mass spectrometry (If time permits)

DALHOUSIE UNIVERSITY

Approximate Projected Schedule (Subject to Change)

Monday	Tuesday	Wednesday	Thursday	Friday
January 8-12				
Week 1	Intro/Theory			
January 15-19				
Week 2	Intro/Theory			
January 22-26				
Week 3	Proton NMR			
January 29 - February 2				
Week 4	Carbon NMR			
February 5-9				
Week 5	Problem Solving			
	Online start		Online end	
February 12-16				
Week 6	Midterm 1		Coupling,2nd order	
February 19-23 Reading Week				
February 26-March 1				
Week 7	2D			
March 4-8				
Week 8	Problem Solving			
Online 2 start		Online 2 end		
March 11-15				
Week 9	Midterm 2		NOE	
March 18-22				
Week 10	NOE/Dynamic NMR		Dynamic NMR	
			Take Home out	
March 25 – 29				
Week 11	F and P NMR			
	Take Home due			
April 1-5				
Week 12	Problem Solving			
	Online 3 start		Online 3 end	

DALHOUSIE UNIVERSITY

University Policies and Statements

Recognition of Mi'kmaq Territory

Dalhousie University would like to acknowledge that the University is on Traditional Mi'kmaq Territory. The Elders in Residence program provides students with access to First Nations elders for guidance, counsel, and support. Visit or e-mail the Indigenous Student Centre at 1321 Edward St or elders@dal.ca. Additional information regarding the Indigenous Student Centre can be found at: https://www.dal.ca/campus_life/communities/indigenous.html

Internationalization

At Dalhousie, 'thinking and acting globally' enhances the quality and impact of education, supporting learning that is "interdisciplinary, cross-cultural, global in reach, and orientated toward solving problems that extend across national borders." Additional internationalization information can be found at: https://www.dal.ca/about-dal/internationalization.html

Academic Integrity

At Dalhousie University, we are guided in all our work by the values of academic integrity: honesty, trust, fairness, responsibility, and respect. As a student, you are required to demonstrate these values in all the work you do. The University provides policies and procedures that every member of the university community is required to follow to ensure academic integrity. Additional academic integrity information can be found at: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Student Accessibility Centre is Dalhousie's centre of expertise for matters related to student accessibility and accommodation. If there are aspects of the design, instruction, and/or experiences within this course (online or in-person) that result in barriers to your inclusion, please contact the Student Accessibility Centre (https://www.dal.ca/campus_life/academic-support/accessibility.html) for all courses offered by Dalhousie with the exception of Truro. For courses offered by the Faculty of Agriculture, please contact the Student Success Centre in Truro (https://www.dal.ca/about-dal/agricultural-campus/student-success-centre.html)

Conduct in the Classroom – Culture of Respect

Substantial and constructive dialogue on challenging issues is an important part of academic inquiry and exchange. It requires willingness to listen and tolerance of opposing points of view. Consideration of individual differences and alternative viewpoints is required of all class members, towards each other, towards instructors, and towards guest speakers. While expressions of differing perspectives are welcome and encouraged, the words and language used should remain within acceptable bounds of civility and respect.

DALHOUSIE UNIVERSITY

Diversity and Inclusion – Culture of Respect

Every person at Dalhousie has a right to be respected and safe. We believe inclusiveness is fundamental to education. We stand for equality. Dalhousie is strengthened in our diversity. We are a respectful and inclusive community. We are committed to being a place where everyone feels welcome and supported, which is why our Strategic Direction prioritizes fostering a culture of diversity and inclusiveness (Strategic Priority 5.2). Additional diversity and inclusion information can be found at: http://www.dal.ca/cultureofrespect.html

Student Code of Conduct

Everyone at Dalhousie is expected to treat others with dignity and respect. The Code of Student Conduct allows Dalhousie to take disciplinary action if students don't follow this community expectation. When appropriate, violations of the code can be resolved in a reasonable and informal manner - perhaps through a restorative justice process. If an informal resolution can't be reached, or would be inappropriate, procedures exist for formal dispute resolution. The full Code of Student Conduct can be found at: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

Fair Dealing Policy

The Dalhousie University Fair Dealing Policy provides guidance for the limited use of copyright protected material without the risk of infringement and without having to seek the permission of copyright owners. It is intended to provide a balance between the rights of creators and the rights of users at Dalhousie. Additional information regarding the Fair Dealing Policy can be found at: https://www.dal.ca/dept/university_secretariat/policies/academic/fair-dealing-policy-.html

Originality Checking Software

The course instructor may use Dalhousie's approved originality checking software and Google to check the originality of any work submitted for credit, in accordance with the Student Submission of Assignments and Use of Originality Checking Software Policy. Students are free, without penalty of grade, to choose an alternative method of attesting to the authenticity of their work and must inform the instructor no later than the last day to add/drop classes of their intent to choose an alternate method. Additional information regarding Originality Checking Software can be found at: https://www.dal.ca/dept/university_secretariat/policies/academic/student-submission-of-assignments-and-use-of-originality-checking-software-policy-.html

Student Use of Course Materials

Course materials are designed for use as part of this course at Dalhousie University and are the property of the instructor unless otherwise stated. Third party copyrighted materials (such as books, journal articles, music, videos, etc.) have either been licensed for use in this course or fall under an exception or limitation in Canadian Copyright law. Copying this course material for distribution (e.g. uploading to a commercial third-party website) may lead to a violation of Copyright law.

DALHOUSIE UNIVERSITY

Student Resources and Support

University Policies and Programs

Important Dates in the Academic Year (including add/drop dates): http://www.dal.ca/academics/important_dates.html
Classroom Recording Protocol: https://www.dal.ca/dept/university_secretariat/policies/academic/classroom-recording-protocol.html
Dalhousie Grading Practices Policies: https://www.dal.ca/dept/university_secretariat/policies/academic/grading-practices-policy.html
Grade Appeal Process: https://www.dal.ca/campus_life/academic-support/grades-and-student-records/appealing-a-grade.html
Sexualized Violence Policy: https://www.dal.ca/dept/university_secretariat/policies/health-and-safety/sexualized-violence-policy.html
Scent-Free Program: https://www.dal.ca/dept/safety/programs-services/occupational-safety/scent-free.html

Learning and Support Resources

General Academic Support – Advising (Halifax): https://www.dal.ca/campus_life/academic-support/advising.html
General Academic Support – Advising (Truro): https://www.dal.ca/about-dal/agricultural-campus/ssc/academic-support/advising.html
Student Health & Wellness Centre: https://www.dal.ca/campus_life/health-and-wellness.html
On Track (helps you transition into university, and supports you through your first year at Dalhousie and beyond): https://www.dal.ca/campus_life/academic-support/On-track.html
Indigenous Student Centre: https://www.dal.ca/campus_life/communities/indigenous.html
Indigenous Connection: https://www.dal.ca/about-dal/indigenous-connection.html
Elders-in-Residence (The Elders in Residence program provides students with access to First Nations elders for guidance, counsel, and support. Visit the office in the Indigenous Student Centre or contact the program at elders@dal.ca or 902-494-6803: https://cdn.dal.ca/content/dam/dalhousie/pdf/academics/UG/indigenous-studies/Elder-Protocol-July2018.pdf
Black Student Advising Centre: https://www.dal.ca/campus_life/communities/black-student-advising.html
International Centre: https://www.dal.ca/campus_life/international-centre.html
South House Sexual and Gender Resource Centre: https://southhousehalifax.ca/about/
LGBTQ2SIA+ Collaborative: https://www.dal.ca/dept/vpei/edia/education/community-specific-spaces/LGBTQ2SIA-collaborative.html
Dalhousie Libraries: http://libraries.dal.ca/
Copyright Office: https://libraries.dal.ca/services/copyright-office.html
Dalhousie Student Advocacy Services: https://www.dsu.ca/dsas?rq=student%20advocacy

Dalhousie Ombudsperson: https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html
Human Rights and Equity Services: https://www.dal.ca/dept/hres.html
Writing Centre: https://www.dal.ca/campus_life/academic-support/writing-and-study-skills.html
Study Skills/Tutoring: http://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html
Faculty of Science Advising Support: https://www.dal.ca/faculty/science/current-students/undergrad-students/degree-planning.html

Safety

Biosafety: http://www.dal.ca/dept/safety/programs-services/biosafety.html
Chemical Safety: https://www.dal.ca/dept/safety/programs-services/chemical-safety.html
Radiation Safety: http://www.dal.ca/dept/safety/programs-services/radiation-safety.html
Laser Safety: https://www.dal.ca/dept/safety/programs-services/radiation-safety/laser-safety.html