DALHOUSIE UNIVERSITY

Organic Structure Determination
Chemistry 4402
Winter 2021

Instructor: Professor Norm Schepp, nschepp@dal.ca
Lectures: Asynchronous, online; tutorials, synchronous Thursdays, 10:05 am to 11:25 am (AST)

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; CHEM 3401 is strongly recommended. Chem 5402 is crosslisted for graduate students. Credit cannot be obtained for both 4402 and 5402.

Course Objectives/Learning Outcomes

- ability to interpret spectroscopic data for compound identification.

Course Materials

- **Lectures** will be posted at the beginning of each week according to the schedule given below.
- **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.
- **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 quizzes and the final examination.

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Course Assessment

Assignment 1	January 22 out – January 27 in (noon deadline)	5 %
Assignment 2	February 5 out - February 10 in (noon deadline)	7 %
Assignment 3	February 26 out – March 3 in (noon deadline)	10 %
Assignment 4	March 12 out - March 17 in (noon deadline)	13 %
Assignment 5	March 26 out – March 31 in (noon deadline)	15 %
Final Exam	3 hr, online, during exam schedule	50 %

A minimum grade of 50% is required in order to pass the course.

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

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)		

All chemistry courses, unless stated otherwise, have a minimum grade requirement of C- for their prerequisite chemistry courses. Students with grades below C- in the prerequisite chemistry courses can only register with the permission of the instructor for the course.

Course Policies

Office hours.

Send me an email to arrange an appointment for a Teams meeting when you have questions.

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

Unless an acceptable excuse (such illness, personal or family emergency, etc.) is communicated to me prior to or within two days after a deadline, late or missed assignments will be given a grade of zero (0). If you are excused for an assignment, its value will be added to the next assignment. For example, if you are excused from Assignment 1 worth 5%, its value will be added to the next assignment so Assignment 2's value will be 12% (7% + 5%). If you are excused from Assignment 5, the final exam will be worth 65%.

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

You are required to complete assignments on your own, without assistance from other classmates or from online help websites. Cheating websites like CHEGG will be monitored.

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Course Content

This class will teach the use of spectroscopic methods to determine the structures of organic compounds. 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 some 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 (in almost random order):

- 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)

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Projected Schedule (Subject to Change)

	Beginning of week lecture available online	Wednesday	Thursday 10 to 11:30 Teams Q&A	Friday
January 6 – 8 No lecture				
January 11-15				
Week 1	Intro			
January 18-22				
Week 2	Intro		Teams Q&A	Quiz 1 out
January 25-29				
Week 3	Proton NMR	Quiz 1 in	Teams Q&A	
February 1-5				
Week 4	Problem Solving		Teams Q&A	Quiz 2 out
February 8-12				
Week 5	Carbon NMR	Quiz 2 in	Teams Q&A	
February 15-19				
February 22-26				
Week 6	Coupling,2nd order		Teams Q&A	Quiz 3 out
March 1-5				
Week 7	Problem Solving	Quiz 3 in	Teams Q&A	
March 8-12				
Week 8	2D		Teams Q&A	Quiz 4 out
March 15-19				
Week 9	NOE	Quiz 4 in	Teams Q&A	
March 22-26				
Week 10	Problem Solving		Teams Q&A	Quiz 5 out
March 29 – April 1				
Week 11	F and P NMR	Quiz 5 in	Teams Q&A	
Exam Period April 10 - 23				

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Faculty of Science Course Syllabus (Section B)

Winter 2021

Chem 4402/5402

University Policies and Statements

This course is governed by the academic rules and regulations set forth in the University Calendar and by Senate

Missed or Late Academic Requirements due to Student Absence

As per Senate decision instructors may not require medical notes of students who must miss an academic requirement**, including the final exam**, for courses offered during fall or winter 2020-21 (until April 30, 2021). Information on regular policy, including the use of the Student Declaration of Absence can be found here: **https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.html.**

Academic Integrity

At Dalhousie University, we are guided in all of our work by the values of academic integrity: honesty, trust, fairness, responsibility and respect (The Center for Academic Integrity, Duke University, 1999). As a student, you are required to demonstrate these values in all of 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.
Information: https://www.dal.ca/dept/university_secretariat/academic-integrity.html

Accessibility

The Advising and Access Services Centre is Dalhousie's centre of expertise for student accessibility and accommodation. The advising team works with students who request accommodation as a result of a disability, religious obligation, or any barrier related to any other characteristic protected under Human Rights legislation (Canada and Nova Scotia).
Information: https://www.dal.ca/campus_life/academic-support/accessibility.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.
Code: https://www.dal.ca/dept/university_secretariat/policies/student-life/code-of-student-conduct.html

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
Statement: http://www.dal.ca/cultureofrespect.html

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 (1321 Edward St) (elders@dal.ca).
Information: https://www.dal.ca/campus_life/communities/indigenous.html

Important Dates in the Academic Year (including add/drop dates)

https://www.dal.ca/academics/important_dates.html

University Grading Practices

https://www.dal.ca/dept/university_secretariat/policies/academic/grading-practices-policy.html

Student Resources and Support

Advising

General Advising https://www.dal.ca/campus_life/academic-support/advising.html

Science Program Advisors: https://www.dal.ca/faculty/science/current-students/academic-advising.html

Indigenous Student Centre: https://www.dal.ca/campus_life/communities/indigenous.html

Black Students Advising Centre: https://www.dal.ca/campus_life/communities/black-student-advising.html

International Centre: https://www.dal.ca/campus_life/international-centre/current-students.html

Academic supports

Library: https://libraries.dal.ca/

Writing Centre: https://www.dal.ca/campus_life/academic-support/writing-and-study-skills.html

Studying for Success: https://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html

Copyright Office: https://libraries.dal.ca/services/copyright-office.html

Fair Dealing Guidelines https://libraries.dal.ca/services/copyright-office/fair-dealing.html

Other supports and services

Student Health & Wellness Centre: https://www.dal.ca/campus_life/health-and-wellness/services-support/student-health-and-wellness.html

Student Advocacy: https://dsu.ca/dsas

Ombudsperson: https://www.dal.ca/campus_life/safety-respect/student-rights-and-responsibilities/where-to-get-help/ombudsperson.html

Safety

Biosafety: https://www.dal.ca/dept/safety/programs-services/biosafety.html

Chemical Safety: https://www.dal.ca/dept/safety/programs-services/chemical-safety.html

Radiation Safety: https://www.dal.ca/dept/safety/programs-services/radiation-safety.html

Scent-Free Program: https://www.dal.ca/dept/safety/programs-services/occupational-safety/scent-free.html