

Organic Structure Determination

Chemistry 4402

Winter 2019

Instructor: Professor Norm Schepp, Room 212 and Room 411, nschepp@dal.ca

Lectures: Chemistry Building, Room 223, Tuesday and Thursday, 10:05 to 11:25

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

- **There is no textbook for this class.** Occasionally, course materials will be available on the Brightspace class website.
- **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 in-class tests, the take-home problem and the final examination.

Course Assessment

In Class Test 1, Tuesday, Jan 22
In Class Test 2, Tuesday, Feb 5
In Class Test 3, Tuesday, Feb 26
Take-Home Problem, Mar 5 – 12
In Class Test 4, Tuesday, Mar 26

TWO OPTIONS: The option that gives the higher overall mark will be applied.

1

Best three of four tests	36% (12% each)
Take-Home Problem, Mar 5 – 12	14%
Final examination (3 hours)	50%
Total	100%

2

Best three of four tests	27% (9% each)
Take-Home Problem, Mar 5 – 12	13%
Final examination (3 hours)	60%
Total	100%

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

The term tests (about 45 minutes, during regularly scheduled class time) and the final examination are all “closed book.” The final examination (time and place to be scheduled by the Registrar) will be a three-hour exam and will cover the whole course.

If one in-class test is missed, the remaining three tests will be used to calculate the final, overall mark. There will be no make-up in-class tests. If a student misses two in-term tests, or fails to hand in the take-home problem, a grade of "F" will be awarded.

A take-home problem will be distributed on March 5, and is to be returned at the beginning of class on March 12. This problem is to be done completely on your own.

Students who are ill for the final exam and produce a proper medical certificate will have an opportunity to write a make-up exam. (See the University Regulations published in the most recent undergraduate calendar).

For the final mark, *if all four in-class tests have been written* the in-class test with the lowest mark will be dropped. (This is *your* lowest mark, not the test with the lowest average

mark.) If you wrote only three tests then the marks on all three tests will be used to calculate your overall mark.

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.

I am often available in the Chemistry Chair's office, so you may just drop by and see if I am free. However, I have lots of administrative duties (and meetings), some research duties, as well as some seminar and PhD examination commitments, and these commitments don't allow me to set regular office hours. Feel free to email me if you want to make an appointment at a specific time.

Email.

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

Cancelled Classes.

In the case of a weather-related closure of the University, a DalAlert email will be sent to all students, faculty and staff. Other information can be found at www.dal.ca/storm.html. In the event that Chem 4402 needs to be cancelled, notification will be sent by email and a notice will be placed on the door to the classroom.

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 ^1H and ^{13}C NMR. Almost everything that will be discussed can be done with the facilities in this Department. "Operation of the NMR spectrometers" mentioned in the course description means advice on obtaining useful spectra, not the actual commands for the running of the instruments. (This sort of training is available through our NMR facility and is obtained in conjunction with research projects.) 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. 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 ^1H and ^{13}C NMR (some ^{15}N , ^{19}F and ^{31}P NMR)
 - Issues of NMR spectral complexity: first and second order spectra
 - 1D ^{13}C NMR spectra as well as SFORD, APT, DEPT
 - 2D NMR spectra including the use of gradient pulses (COSY, HETCOR, TOCSY, HSQC, HMQC, HMBC, INADEQUATE)
 - NMR Relaxation phenomena
 - NOE: its measurement and exploitation
 - Dynamic NMR
 - Overview of the useful aspects of IR
 - Mass spectrometry
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**Faculty of Science Course Syllabus (Section B)
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

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

Missed or Late Academic Requirements due to Student Absence (policy)

https://www.dal.ca/dept/university_secretariat/policies/academic/missed-or-late-academic-requirements-due-to-student-absence.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>