

Physical Organic and Spectroscopy CHEM3404 (Online) Fall 2020

Instructor(s):

Professor Frances Cozens, Virtual Office frances.cozens@dal.ca. Principle Instructor, day-to-day class inquires and all administrative matters for the CHEM3404 lectures.

Office Hours Via Teams – scheduled hours (TBA) or by appointment. You are welcome to e-mail Dr. Cozens if you would like to make an appointment for a specific time. Please put CHEM3404 in the subject line.

Dr. Reinaldo Moya-Barrios, Virtual Office rbarrios@dal.ca. Laboratory instructor, day-to-day supervision and all administrative matters for the CHEM3404 laboratories. Office Hours Via Teams – scheduled hours (TBA) or by appointment. You are welcome to e-mail Dr. Moya-Barrios if you would like to make an appointment for a specific time. Please put CHEM3404 in the subject line.

Lectures: Weekly lecture material including readings and videos presentations will be uploaded to Brightspace, asynchronous format. The class will be formatted with weekly uploads to Brightspace.

Laboratories: Weekly laboratory material will be uploaded to Brightspace, asynchronous format. Synchronous Teams meetings will be scheduled throughout the term in the regular scheduled Monday and Thursday, 1:35 - 5:25 pm timeslot.

Lectures and tutorials: Synchronous Teams meetings will be scheduled throughout the term in the Monday, Wednesday or Friday, 11:35 am - 12:25 pm timeslots.

The following pages constitute the syllabus for this course, CHEM3404. You can consider the syllabus to be a contract, which delineates responsibilities and expectations for both the students and the teaching team. You should review the syllabus thoroughly, refer to it as necessary throughout the term, and contact the instructor with any questions and/or concerns you may have.

Course Description: Credit hours: 3 Format: Lecture and Laboratories Online synchronous and asynchronous. This course provides an introduction to spectroscopic techniques with an emphasis on proton and carbon NMR spectroscopy. Concepts in physical organic chemistry are also described and are used to explain structure reactivity relationships. The laboratory will focus on learning about the tools used in compound identification (spectroscopy) and data analysis (physical organic chemistry).

Course Prerequisites:

PREREQUISITES: CHEM 2401.03/2402.03 or equivalent (grade of C- or better).

Course Objectives/Learning Outcomes:

1) Spectroscopy:

- understanding and utilizing IR spectroscopy, UV spectroscopy, High Resolution Mass Spectrometry and Proton and Carbon NMR spectroscopy
- having the ability to interpret spectroscopic data for organic compound identification
- having the ability to identify complex NMR data for compound identification
- the laboratory will be utilized to enhance the learning outcomes

2) Physical Organic Chemistry:

- understand the effect of substituents in organic chemistry
- predict mechanisms and transition state structures
- fully appreciate complexities of nucleophilic substitution reactions
- recall structures and properties of select reactive intermediates
- the laboratory will be utilized to enhance the learning outcomes

Course Materials:

Lectures:

- Class video lectures will be available on the Brightspace class website. The class will be formatted into
 weekly segments. NOTE: Lecture notes and videos subject to change. The latest version of the class
 notes and video lectures will be posted to Brightspace. All material posted to Brightspace is under
 copyright rules @ 2020 and cannot be further distributed without prior consent of the course Instructors.
- Brightspace and Microsoft Teams Video conferencing will be utilized for both the lecture and laboratory components of this class. Since all the class material will be posted online along with online evaluations, you will need access to a computer and a reliable internet connection to complete this class.
- Textbook "Advanced Organic Chemistry, 5th Edition, Part A: Structure and Mechanisms", by Carey and Sundberg, Springer, 2007 is a valuable reference book for this class. This book is available online to Dalhousie students in the library or logged-in via VPN. This book has a great deal of useful information and should be part of student resources. Excerpts from this book will be uploaded as weekly reading for the Structure and Mechanisms part of the class.

http://lib.myilibrary.com.ezproxy.library.dal.ca/Open.aspx?id=4318

- **Textbook** "Introduction to Spectroscopy, 4th or 5th Edition", by Donald L. Pavia, Gary M. Lampman, George S. Kriz and James A. Vyvyan, 2009 or 2014. This book has a great deal of useful information. Excerpts from this book will be uploaded as weekly reading for the Spectroscopy part of the class.
- Practice Problems Practice problems will be available on Brightspace for both Physical Organic Chemistry and Spectroscopy modules. These problems are extremely important to complete for the successful completion of CHEM3404. Answers will also be posted to Brightspace. Some problems will be explained via video presentations.
- **Tutorial Help** Each student will be assigned a Teaching assistant that will be available to help with the material presented in CHEM3404. Synchronous tutorials will be scheduled throughout the term for help with presented material.

Laboratory:

- All laboratory activities will be online.
- All work must be independent.
- Presentation of the lab material will be asynchronous.
- Each week there will synchronous online office hours where you can meet with your Instructor and discuss the material being presented in the lab modules, lab report questions and questions related to data analysis in general. The rest of the week the Instructor will be available via email.
- All the necessary laboratory information will be available in the CHEM3404 Brightspace site or in the indicated websites (see list below).
- The laboratory work will be divided in seven (7) modules.
- Module 1 will be introductory and will provide you with fundamental tools that you will need this semester, such as how to process raw NMR data using TopSpin, how to conduct a proper literature search and how to prepare a formal lab report.
- Modules (2 to 7) will have a similar structure. The content and instructions for each of these modules
 will be posted online on the Monday of the scheduled week in the form of slide presentations. This
 material will be accompanied with videos that will facilitate your understanding of a particular topic or
 procedure.
- Modules 2 to 7 will be evaluated in two ways:
 - 1. Each module will have an assessment quiz that must be completed within a week of the day the module was first posted.
 - 2. The data provided in each module will be analyzed and discussed in lab reports that will be due two weeks after the module was posted. More details on lab reports can be found in Brightspace.

Websites:

Databases

- Web of Science Citation Databases (Chemistry search; Dalhousie library)
 http://apps.webofknowledge.com/UA_GeneralSearch_input.do?product=UA&search_mode=GeneralSearch&SID=4CqG4ooilR25p7YLkk2&preferencesSaved=
- Scifinder Scholar (chemistry search; Dalhousie library) https://scifinder.cas.org/scifinder/login
- Spectral Database for Organic Compounds http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

General Chemical Information

- Chemical Institute of Canada (www.cheminst.ca/)
- Royal Society of Chemistry (www.rsc.org)
- American Chemical Society (www.acs.org & pubs.acs.org)

Course Assessment:

Total	100%
Laboratory	20%
Final examination	30%
Two online assignments	15% each
Online Quizzes	20% total

Dates of online assignments:

Online quizzes will be assigned throughout the term. 10% weight for each module.

Assignment 1 (end of module 1) handed out October 14, 2020 with 48 hours to complete, due Oct. 16, 2020.

Assignment 2 (end of module 2) handed out November 25, 2020 with 48 hours to complete, due Nov. 27, 2020.

Final Examination (time and place to be scheduled by the Registrar) will be a three-hour exam and will cover the entire course.

Other course requirements

A minimum grade of 11/20 is required in the laboratory portion of CHEM3404 to pass the class.

Notes:

Synchronous components will be offered but attendance will not be required.

Final examination will be a three-hour timed examination.

Final examination will be held in the regular exam scheduled time.

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)		

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

Emergencies

Missed or Late Academic Requirements due to Student Absence. Dalhousie students are asked to take responsibility for their own short-term absences (3 days or less) by contacting their instructor by email prior to the academic requirement deadline or scheduled time and by submitting a completed Student Declaration of Absence to their instructor in case of missed or late academic requirements. Only 2 separate Student Declaration of Absence forms may be submitted per course during a term. read more:

https://cdn.dal.ca/content/dam/dalhousie/pdf/dept/university_secretariat/policy-repository/StudentAbsenceRegulation(OCT2017)v2.pdf)

Evaluations. Quizzes will be available for each module and scheduled during the term. The online assignments will be due 48 hours after released. If you are experiencing illness, please submit a student declaration of absence and the due date will be adjusted accordingly. All work must be completed in the class.

The three-hour final examination will cover the entire course. A student may write a make-up final examination if the final examination was missed with a justifiable reason. The date and time of the make-up examination will be decided a few days after the CHEM3404 final examination has been written and will be at the end of the regular examination period. The University policy is that final examinations are not returned to students.

Independent work. All graded work in CHEM3404 (class and laboratory material) must be done independently by each student enrolled in the class. Online resources can be used for all graded work, except 'cheating' websites such as CHEGG.COM.

Copyright @. All material posted online for CHEM3404 is strictly copyrighted. No class material can be distributed in any way to a third party. Upon investigation via University protocols and found to participate in the uploading of any material to a third party or sharing with anyone not enrolled in the class will lead to a **mark of 'F' for CHEM3404**. All work must be the student's independent and individually prepared work. Student work that is not independently done will receive a **mark of 0 on the submitted material**. Utilizing online resources is allowed.

Email. It is your responsibility to read your Dalhousie email, as class notifications may be sent by email. For any correspondence in CHEM3404 please use email to contact Dr. Cozens or Dr. Moya-Barrios.

Delayed Classes. In the case of a weather-related closure, internet or power interruptions, online content may be delayed.

Course Content:

Lectures. The following topics are expected to be covered in CHEM3404 and are listed below. Class video lectures will be available on Brightspace.

Part 1: 6 week module on Spectroscopy. Topics to be included are:

UV-Vis Spectroscopy

IR Spectroscopy

High Resolution Mass Spectrometry for molecular formula determination

Proton and Carbon NMR Spectroscopy

Part 2: 6 week module on Physical Organic Chemistry. Topics to be included are:

Substituent effects

Hammett equations and other free energy relationships.

Energy Diagrams

Transition state structure and the Hammond Postulate.

Kinetic Isotope Effects

Origin and use in determining reaction mechanisms and transition state structure.

Nucleophilic Substitution Reactions

S_N1 and S_N2 reactions, leaving group ability, nucleophile ability.

Carbocations

Reactivity and stability.

Other reactive Intermediates

Chemistry of radicals, carbenes and carbanions

Any other physical organic topic

Faculty of Science Course Syllabus (Section B)

CHEM3404 Fall 2020

Intermediate Organic Chemistry Physical Organic and Spectroscopy

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 <u>may not require medical notes</u> of students who must miss an academic requirement, **including the final exam**, for courses offered during fall or winter 2020-21 (<u>until April 30, 2021</u>). 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'kmag 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 email 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

 $\textbf{Studying for Success:} \ \underline{\text{https://www.dal.ca/campus_life/academic-support/study-skills-and-tutoring.html}}$

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