

CONCORDIA UNIVERSITY
DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY
CHEMISTRY 293 - SPECTROSCOPY AND STRUCTURE OF ORGANIC COMPOUNDS

This course aims at presenting an introduction to the techniques used to characterize organic molecules. UV-VIS, IR, NMR and MS are the four main spectrometric methods covered in this class.

COURSE FORMAT: Lecture and Laboratory.

INSTRUCTORS: Sébastien Robidoux Lec. 51 : M/W CC-115 10:15-11:30
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OFFICE HOURS: Monday 13H00-15H00 Wednesday 13H00-15H00

AUDIENCE: This course is part of the core component for students enrolled in Chemistry and Biochemistry programs at Concordia.

CONTENT: The course is divided into 5 topics covered over 22 lectures.

1. Elemental Analysis and Molar Mass Determination (2 lectures)
2. Ultra-Violet and Visible Spectroscopy (3 lectures)
3. Infra-Red Spectroscopy (3 lectures)
4. Nuclear Magnetic Resonance Spectroscopy (10 lectures)
5. Mass Spectrometry (4 lectures)

The first section on elemental analysis and molar mass determination will present to the students a brief review of elemental analysis and colligative properties seen previously in general chemistry. A quick introduction of the 4 major characterization methods (UV-VIS, IR, NMR and MS) was already presented in the prerequisite course CHEM 222. The theory and practical applications of the same 4 methods will be covered in this course.

This course is officially a physical chemistry course. You will therefore have to manipulate some equations, especially equations dealing with energy. There is also an organic chemistry component. Functional group chemistry and simple theory about structure of organic compound should have been mastered in CHEM 222 and 221.

You are responsible for all the material present in Chapter 1 to 11 except for sections 6.9, 6.10, 7.3, 7.4, and 8.8-12. For chapter 9, only 9.1 and 9.6-9.8 will be covered and tested. I will **NOT** discuss all the sections of these chapters in class, especially the sections talking about the data and numbers for all functional groups. You do not have to memorize all of these numbers, but you have to be familiar with them. I will focus on theory and important practical applications and I will do a few problems in class.

STATEMENT OBJECTIVES: This course should help students

- to know the name and the structure of most functional groups in organic chemistry. (Intermediate to Advanced level)
- to characterize and identify simple organic molecules. (Intermediate level)
- to calculate the energy for the transitions in the spectroscopic methods studied (UV-Vis, IR, and NMR) (Basic level)
- to calculate the population ratio in the excited and ground states in the spectroscopic methods studied (UV-Vis, IR, and NMR) (Basic level)
- to evaluate which technique is best to identify a specific compound. (Intermediate level)

- to analyze the fragmentation pattern and the isotopic ratio data of a compound in MS. (Intermediate level)
- to analyze a splitting pattern in NMR. (Intermediate level)
- to explain the shift and intensity of bands or peaks in the spectroscopic methods studied (UV-Vis, IR, and NMR) (Basic level)
- to use 2D NMR techniques (Basic Level)

ACCESSIBILITY: In order to make the course more accessible, I am committed to reducing barriers that students might have. This will be done using multiple ways to ensure inclusion. Students who know that this course might offer challenges are invited to contact me to discuss their concerns and the possible means and strategies that can be applied to attain the objectives stated previously. However, if you require that an accommodation plan be established to help reduce the barriers you face as a result of a disability condition (including mental health conditions as well as chronic and temporary medical conditions) then you are requested to meet with the Access Centre for Students with Disabilities in a timely fashion.

ACSD Contact information: acsinfo@concordia.ca; 514-848-2424 ext. 3525; SGW Campus, GM-300.00

TEXTBOOK: Introduction to Spectroscopy by D.L.Pavia, G.M. Lampman, G.S. Kriz and J.R. Vyvyan, 5th Edition, CENGAGE Learning, 2015 is the required textbook for the theory component of the course. You can buy a hard copy at the bookstore. It would be useful to have a standard textbook of organic chemistry, such as Organic Chemistry by Jones, Bruice, or any other ones. Reading and problems are assigned in the Pavia's book.

A laboratory coursepack: **Spectroscopy and Structure**, must also be purchased from the University Bookstore.

EXAMINATIONS: There will be **FOUR** formal examinations:

1. Test 1 **in CLASS 1 hour and 15 minutes** for four questions on molecular formula determination, UV-Vis, and IR: Lecture 51 June 11, 2018
2. Test 2 **in CLASS 1 hour and 15 minutes** for four questions on NMR
Lecture 51 July 25, 2018

If a student is absent from a test, he/she must produce a written excuse appropriately signed (i.e. by a doctor, or an employer) on the appropriate letterhead paper. This letter must be delivered to the instructor **NO LATER THAN ONE (1) WEEK AFTER THE TEST**. The Department determines the validity of the absence. If there is no valid excuse, the student will receive a mark of zero for the test. There is no makeup test. In case of a valid excuse, percentage grade is transferred unto the final exam.

3. A final examination, between August 16 and August 21, 2018 arranged by the Examinations Office.
4. A laboratory exam on **MOODLE** for **30 minutes** for 10 multiple choice questions and 5 short answer questions. It must be done between August 3 18H30 and August 6 18H30.

SURPRISE QUIZ: 5 or 6 surprise quizzes will be given during the term. Each of them will include 1 or 2 simple questions related to the two previous lectures. Students will have between 5 and 10 minutes to complete the quiz. No surprise quiz will be given during the lecture before or after a test. The worst grade will be dropped in order to count the best 4 or 5 grades. Attendance will be judged on the number of quizzes completed. If you feel that the format of the quiz will not give you a fair opportunity at showing your knowledge, speak with the professor.

COURSE GRADE: The final grade of the course is based on the marks obtained in the examinations, quizzes and the laboratory marks. The composition of the final grade is as follow:

Surprise quizzes (best 4-5 out of 5-6)	10%
Attendance	5%
Test 1	12.5%
Test 2	12.5%
Final exam	35%
Lab reports	15%
Lab examination	10%

	100%

Separate minimum passing marks are required for the theory (weighted average of the two tests, the final exam, the attendance and the surprise quizzes), for the lab (weighted average of the lab reports and the lab exam) and for the lab exam. Minimum passing marks for the lab exam and the theory is 50% (D) and for the lab is 60% (C-).

Letter grades will be assigned according to the following criteria:

A+: 90.00-100.00	A: 85.00-89.99	A-: 80.00-84.99
B+: 76.67-79.99	B: 73.33-76.66	B-: 70.00-73.32
C+: 66.67-70.00	C: 63.33-66.66	C-: 60.00-63.32
D+: 55.00-60.00	D: 50.00-55.00	F: see previous paragraph

MANDATORY QUIZ AND SEMINAR

As part of this course, you are **required** to i) attend a Chemistry and Biochemistry Departmental Seminar on the academic conduct code and the appropriate use of information sources and ii) pass the online quiz associated with this seminar (the passing grade for the quiz is 100%). (**Note:** This is **not** the University's quiz you may have been asked to take when you first registered and logged into the myConcordia portal; the one you must take is similar, but graded by the Department of Chemistry and Biochemistry, and you cannot take it until after you have attended the seminar.) The aim of this seminar is to clarify the academic conduct code in terms of what practices will be considered unacceptable with regards to work submitted for grading in Chemistry and Biochemistry courses. **You are only exempt from repeating the seminar and the quiz if you have done both in Summer 2013 or more recently,*** otherwise you are required to repeat both this term. This short seminar (1 hour) will be held at the following time (note that late-comers will not be admitted):

Date	Time	Place
Friday, May 11	17:45-18:45 pm	SP S110

If you do not complete this course requirement, your final grade for the course may be lowered by one full letter grade with an incomplete notation until such time as this requirement is completed. Please refer to the undergraduate calendar (section 16.3.6) for details on removal of an incomplete notation.

* You are exempt if you can locate your ID in the pdf file located on the CHEM 101 Moodle site (for guest login, go to: <http://moodle.concordia.ca/moodle>, Arts and Science, Chemistry and Biochemistry, Specialized Chemistry Sites, CHEM 101, look under FAQ).

PLAGIARISM AND OTHER FORMS OF ACADEMIC DISHONESTY:

The academic code of conduct can be found in section 17.10 of the academic calendar (<http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html>). Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. The mandatory seminar is a clear and fair opportunity to learn what our

faculty regards as academic misconduct. Failure to take part in this learning opportunity and thus ignorance of these regulations is no excuse and will not result in a reduced sanction in any case where academic misconduct is observed.

COURSE NUMBER & SECTIONS: Make it a point to remember the *course number*, your *lecture section number* and your *lab section number* for the duration of the course. This information will be required frequently later when you have to fill in your answer books during examinations and when submitting lab reports, etc., to ensure that your grades are correctly recorded.

LABORATORY INFORMATION: Laboratory Coordinator: Mr Alexey Denisov, SP-S185.01, Tel. 848-2424 ext. 5302. Email: Alexey.denisov@concordia.ca Chem. 293 Laboratories are located at SP-320. **Laboratories start the week of Monday, May 7, 2018.** All students must attend the section for which they are registered during this week. All questions on matters related to the lab organization should be addressed to Mr. Denisov.

Laboratory performance is graded based on the quality of the experimental work, the laboratory reports and a laboratory exam.

Do not expect a particular laboratory experiment to be directly related to the material covered in the lectures of the preceding week. **CONSIDER THE LABORATORY WORK AS AN INDEPENDENT AND ADDITIONAL LEARNING EXPERIENCE.**

LABORATORY COURSEPACK: The lab manual for the course is: **SPECTROSCOPY AND STRUCTURE**. This is available from the University Bookstore, as are other items such as lab coats and safety glasses which are mandatory. You also need to buy a lab note book: **STUDENT LAB NOTEBOOK-CARBONLESS** from the bookstore.

LAB CONTENT: The laboratory component of the course is divided into 8 experiments spread over 10 weeks.

- Experiment 1. Identification of an Unknown Organic Compound through Spectroscopy
- Experiment 2. Ultraviolet Spectroscopy I: Use of Empirical Rules for the Calculation of λ_{\max} in α,β -Unsaturated Carbonyl Compounds
- Experiment 3. Infrared Spectroscopy I: Detailed Analysis of Aspirin and Salicylic Acid
- Experiment 4. NMR Spectroscopy I: Analysis of a Keto-Enol Equilibrium
- Experiment 5. Using Computed Spectroscopic Data. Dry Lab.
- Experiment 6. Ultraviolet Spectroscopy II: Determination of an Isosbestic Point in the Hydrolysis of Aspirin
- Experiment 7. Infrared Spectroscopy II: Study of Inter- and Intramolecular Hydrogen Bonding in Nitrophenols
- Experiment 8. NMR Spectroscopy II: Assessing J-coupling in Aspirin and Salicylic Acid

The objective of the experiments is to get yourself familiarize with the instrumentation used in UV-Vis, IR and NMR spectroscopies. You will be exposed to simple and advanced instrumentation, as well as some concepts not seen in class. For some experiments, you will be judged on the quality of the spectra obtained. There will be a full lab report to write for every experiment. You are invited to read the coursepack or the Moodle lab website for more information.

LAB EXEMPTIONS: Students who are repeating the course, having passed the lab component within the past two (2) years, may be eligible for a lab exemption. Applications for the exemption (forms available in SP201.01) must be completed by the end of the first week of term (*i.e.* prior to the start of the laboratory); late applications will not be accepted. Signed and completed forms are to be returned to

Hilary Scuffell, (SP 275.01). Students MUST register for the appropriate lab exemption lab/tutorial section; students registered in any other lab/tutorial sections will be required to complete the lab portion of the course (NO EXCEPTIONS).

LABORATORY INSTRUCTORS (TEACHING ASSISTANTS): Each laboratory section will have one demonstrator who is a senior undergraduate, a graduate student or a staff member of the department. You must know her or his name, email and the location of his or her room. You will need to contact them later for matters related to your labs.

COURSE WITHDRAWALS: Students who withdraw from the course must also check-out from their laboratory section. Only those students registered in the course may attend the laboratory and receive a grade for lab work.

TYPES OF QUESTIONS

Examinations	Quiz	Test 1	Test 2	Final	Example 1	Example 2
to know the name and the structure of most functional groups in organic chemistry. (Intermediate to Advanced level)	Yes	Yes (2-3)	Yes (2)	Yes (4-5)	Sample Test 1 Question 3	Sample Final 1 Question 6
to characterize and identify simple organic molecules. (Intermediate level)	Yes	Yes (3-4)	Yes (2)	Yes (3-4)	Sample Test 2 Question 3	Sample Final 1 Question 7
to calculate the energy for the transitions in the spectroscopic methods studied (UV-Vis, IR, and NMR) (Basic level)	Yes	Yes (1-2)	Yes (1)	Yes (1-2)	Sample Test 2 Question 1	Sample Final 1 Question 8
to calculate the population ratio in the excited and ground states in the spectroscopic methods studied (UV-Vis, IR, and NMR) (Basic level)	Yes	No	Yes (1)	Yes (1)	Sample Test 2 Question 1	Sample Final 1 Question 8
to evaluate which technique is the best to identify a specific compound. (Intermediate level)	Yes	Yes (1)	Yes (1)	Yes (2-3)	Sample Test 1 Question 3	Sample Final 1 Question 6
to analyze the fragmentation pattern and the isotopic ratio data of a compound in MS. (Intermediate level)	Yes	No	No	Yes (2)	Sample Final 2 Question 2	Sample Final 2 Question 4
to analyze a splitting pattern in NMR. (Intermediate level)	Yes	No	Yes (1-2)	Yes (1)	Sample Test 2 Question 4	Sample Final 2 Question 3
to explain the shift and intensity of bands or peaks in the spectroscopic methods studied (UV-Vis, IR, and NMR) (Basic level)	Yes	Yes (1)	Yes (1)	Yes (1-2)	Sample Test 1 Question 2	Sample Final 1 Question 8
to use 2D NMR techniques (Basic Level)	Yes	No	Yes (1)	Yes (1)	Sample Final 1 Question 7	Sample Final 2 Question 7