CHEM 495 – Advanced Molecular Characterization – Fall 2019 – 3 cred.

1. GENERAL INFORMATION

Course Format	**Lectures**: 13 sessions of 2h30 / week	**Mon**	**18:00–20:30**	**LOY–CC–405**
Instructor	Dr. Xavier OTTENWAELDER Office hours: by appointment	SP–201.19 dr.x@concordia.ca		ext. 8934

2. COURSE DESCRIPTION

This course demonstrates how quantum theory applies to the measurement of absorption and emission spectra of atoms and molecules. The course examines rotational, vibrational, and electronic spectroscopy, photoelectron and related spectroscopies. Lasers and laser spectroscopy. Lectures only.

Prerequisite courses: CHEM 241, 293 and 6 credits of CHEM 300-level courses

3. OBJECTIVES

To provide a solid knowledge of the mode of action of spectroscopic techniques. To use experimental spectroscopic data to analyze and solve real-case chemistry problems.

4. SCHEDULE and OUTLINE

	Chapter topic	A glimpse of the lecture content
I.	**Interaction between Matter and Radiation**	Background on quantum chem: wavefunctions and operators. Absorption and emission of a radiation. Einstein coefficients. Probability of transition. Beer's law. Line shape.
II.	**Rotational Spectroscopy**	Classical and quantum descriptions. Selection rules. Influence of dipole moment (IR), of polarization (Raman).
III.	**Vibrational Spectroscopy**	
IV.	**Electronic Spectroscopy, Fluorescence, Lasers**	Spin and symmetry selection rules. Luminescence. Lasers. Resonance Raman. Two-photon absorption.
V.	**Advanced NMR**	I > ½, natural abundance, 2D techniques.
VI.	**Electron Spin Resonance**	Spin-orbit coupling. g and D tensors. Hyperfine coupling. ZFS.
VII.	**Mössbauer Spectroscopy**	Principles, applications.
VIII.	**Scattering Methods**	EXAFS, Single-crystal X-ray and neutron diffraction.
IX.	**Electroschemistry**	Cyclic voltammetry and examples.

5. MATERIAL

Recommended Textbooks
- J. Michael Hollas, Modern Spectroscopy, 4th ed., 2004 (Wiley)
- Rankin, Mitzel, Morrison, *Structural Methods in Molecular Inorganic Chemistry*, 1st ed., 2013 (Wiley)

6. COURSE FORMAT and GRADING

The final grade will be weighted and calculated as follows:

Problem Sets and In-Class Tests: 40% | Oral/Poster Presentation: 20% | Final Exam: 40%

A grade ≥	0%	50.00	53.33	56.67	60.00	63.33	66.67	70.00	73.33	76.67	80.00	85.00	90.00
and <	50.00	53.33	56.67	60.00	63.33	66.67	70.00	73.33	76.6	80.00	85.00	90.00	100%
gets a:	F	D–	D	D+	C–	C	C+	B–	B	B+	A–	A	A+

To pass CHEM 495, you must obtain at least 50% on the coursework overall.

In the event of extraordinary circumstances beyond the University's control, the content and/or evaluation scheme in this course is subject to change.

If absent from an examination, you must produce a written excuse on letterhead paper appropriately signed (e.g., by a doctor or employer) within one week after the exam. The Department determines the validity of the absence and necessary arrangements will be made. If no valid excuse is produced, the student will receive a **zero** grade for the missed work.

PROBLEM SETS AND MIDTERM EXAMINATION

Problem sets are distributed in class and must be handed in at the beginning of class on the due date (usually 2 weeks thereafter). Late submissions will not be accepted. **Papers slid under an office door will not be graded.**
In-class tests may be announced prior to the class-time at which they are held. A 60-minute period will be allocated towards the completion of the in-class tests, after which teaching in class will resume.

ORAL/POSTER PRESENTATION

Every student is required to present a topic related to the course subject. The format will be either an oral presentation to the class (max 15 min including questions from the class) or a poster presentation (with guest judges). The goal is to cover specific subjects in more detail than will be done during the lectures. The presentation shall address some fundamental or applied aspect(s) of spectroscopy or molecular characterization. The students are required to provide the instructor with an **outline** of their presentation at least **1 week** prior to the presentation. This outline is destined at assessing the progress on literature research related to the topic that will be presented orally. The presentations will be graded based on quality of content, presentation skills, as well as analytical and critical evaluation of the topic.

ACEDMIC INTEGRITY

(Source: http://www.concordia.ca/students/academic-integrity.html)
Please go to the link above and familiarize yourself with what you are supposed to do and what you are supposed to avoid doing.

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 Department of Chemistry and Biochemistry offers a short (1 hour) seminar on the academic conduct code and the appropriate use of information sources which aims to clarify what practices will be considered unacceptable with regards to work submitted for grading in Chemistry and Biochemistry courses. Attendance at this seminar is highly recommended and represents 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. See the Departmental office (SP 201.01) for scheduling (note that late-comers will not be admitted).