

ext. 3279

# CHEM 495 – MODERN SPECTROSCOPY – FALL 2016 – 3 CREDITS

#### **1. GENERAL INFORMATION**

**Course Format** Lectures: 13 sessions of 2h30 / week

Instructor Dr. Rafik Naccache Office hours: by appointment Mon 18:00–20:30 CC 425 LOY

SP-265.20 rafik.naccache@concordia.ca

## 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 molecular symmetry, rotational, vibrational, and electronic spectroscopy, photoelectron and related spectroscopies. Lasers and laser spectroscopy. Lectures only.

Prerequisite courses: CHEM 234, 241, 333

## 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. Molecular Symmetry	Symmetry elements and operations. Group theory.
II. Interaction between Matter and Rad	liation Background on quantum chem: wavefunctions and operators Absorption and emission of a radiation. Einstein coefficients. Probability of transition. Beer's law. Line shape.
III. Rotational Spectroscopy IV. Vibrational Spectroscopy	Classical and quantum descriptions. Selection rules. Influence of dipole moment (IR), of polarization (Raman).
V. Electronic Spectroscopy, Fluoresce Lasers	ence, Spin and symmetry selection rules. Luminescence. Lasers. Resonance Raman. Two-photon absorption.
VI. Electron Spin Resonance	Spin-orbit coupling. g values. Hyperfine coupling. Zero-field splitting. D tensor.

#### 5. MATERIAL

Recommended Textbooks
J. Michael Hollas, Modern Spectroscopy, 4th ed., 2004 (Wiley)
Rankin, Mitzel Morrison, *Structural Methods in Molecular Inorganic Chemistry*, 1<sup>st</sup> ed., 2013 (Wiley)
Atkins, Physical Chemistry 8<sup>th</sup> edition (Oxford) or later

## 6. COURSE FORMAT and GRADING

The final grade will be weighted and calculated as follows:

Proble Mid-ter			20% 20%		ral Pres nal Exa	sentatio Im:	n (15 m	,	20% 40% (dı	uring the	e exam	period)	•
A grade ≥									73.33				
and <	50.00	53.33	10.00	60.00	03.33	00.07	70.00	13.33	76.6	80.00	85.00	90.00	100%
gets a:	F	D–	D	D+	C–	С	C+	В-	В	B+	A–	А	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.

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.

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.

#### MIDTERM

The midterm will take place on the October 31st, 2016. A 60-minute period will be allocated towards the completion of the midterm after which teaching in class will resume.

# ORAL PRESENTATION

Every student is required to present a topic related to the course subject in an oral presentation to the class. The presentation shall not exceed 20 minutes and will be followed by questions from the class. The goal is to cover specific subjects in more detail than will be done during the lectures. The presentation shall address both fundamental <u>and</u> applied aspect(s) of spectroscopy. The instructor will propose a list of topics during class; however, students can also propose topics if they so desire. Students must decide on their topic no later than October 17<sup>th</sup>. If they do not communicate their choice by that date, the instructor will assign a topic to the student. The students are required to provide the instructor with an **outline** of their presentation **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. The presentations will take place between **November 7-21, 2016**.

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

The most common offense under the Academic Code of Conduct is plagiarism, which the Code defines as "the presentation of the work of another person as one's own or without proper acknowledgement."

"Work" here could be material copied word for word from books, journals, internet sites, professor's course notes, etc. It could be material for which the words have been changed but who's phrasing still closely resembles that of the original source. It could be the work of a fellow student, e.g., a lab report completed by another student, or unauthorized data for a lab report. It could be a paper purchased through one of the many available sources. "Plagiarism" does not refer to words alone – it also refers to images, graphs, tables and ideas. "Presentation" is not limited to written work. It also includes computer and artistic works. Finally, if you translate the work of another person into English and do not cite the source, this is also plagiarism.

The Academic Code of Conduct can be found in section 17.10 of the undergraduate calendar (http://www.concordia.ca/academics/undergraduate/calendar/current/17-10.html). Any form of cheating, unauthorized collaboration, copying or plagiarism found in this course will be reported and the appropriate sanctions applied.

As part of CHEM 495, you are required to attend a seminar and pass a quiz on avoiding plagiarism and other forms of academic dishonesty, offered by the Department of Chemistry and Biochemistry. If you have already attended the seminar and achieved 100 % (110 points) on the quiz **within the past five (5) years** (i.e. Fall



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2011 or more recently), you have fulfilled the requirement. The aim of the seminar and quiz is to clarify which practices are considered unacceptable by the Department of Chemistry and Biochemistry. The seminar will be offered during the third week of classes (see below for the times offered); the quiz is online, can be accessed through the MyConcordia portal (click on Powered by Moodle under Course Websites and choose CHEM 101 under Specialized Chemistry Sites; not possible through the guest login!) and can be taken from after the seminar up to the deadline announced on the CHEM 101 site, but preferably as soon as possible. If you do not attend the seminar and/or do not pass the quiz (the passing mark is 100 %), your course grade will be lowered by one full letter grade with an incomplete (INC) notation. Please refer to the academic calendar section 16.3.6 on how to remove the INC and restore the proper course grade.

#### Mandatory Quiz & Seminar

This short seminar (1 hour) will be held at the following times (note that late-comers will not be admitted):

Date (Winter 2016)	Time	Place
Monday, Sept. 26	16:45-17:45	CC-308
Tuesday, Sept. 27	16:45-17:45	HB-130
Wednesday, Sept. 28	16:45-17:45	CC-308
Wednesday, Sept. 28	20:45-21:45	HC-157
Thursday, Sept. 29	16:45-17:45	CC-204
Thursday, Sept. 29	20:45-21:45	HC-157
Friday, Sept. 30	16:45-17:45	CC-310

As space for each of the seminars is limited by the room size, please sign up to your preferred time. Sign-up sheets are available outside SP 201.01 (Departmental office).

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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 (INC) 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).

Good Luck to all and let's have a great semester!!

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