

**CONCORDIA UNIVERSITY
DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

**CHEM 495
ADVANCED MOLECULAR CHARACTERIZATION**

SYLLABUS – Fall 2022

GENERAL INFORMATION

Taken from the undergraduate calendar: “This course presents advanced techniques to characterize the geometric and electronic structures of molecules. This includes spectroscopic (rotational, vibrational, electronic, photoelectron, NMR, EPR, Mössbauer), diffraction and electrochemical methods. The course introduces the techniques and applies them to concrete case studies.” “Includes” in the above means “may include”: the Fall 2022 will only see the first four topics.

Advanced Molecular Characterization (CHEM 495) is a one-term, 3-credit course available to senior undergraduate students. It is offered as a “90” course, and as such is not linked to any specific sub-discipline, analogous to CHEM 293. Prerequisites are CHEM 241 and 293, plus either of CHEM 325 or 341 (and one additional CHEM 300-level course). The Fall 2022 course builds on an introduction to symmetry as it has been covered, e.g., in CHEM 325 or 341, and on UV-Vis and IR basics as covered in CHEM 293.

INSTRUCTOR	Professor H.M. Muchall SP 275.15; heidi.muchall@concordia.ca
COURSE FORMAT	Lectures
LECTURE HOURS	We/Fr 10:15 – 11:30
LOCATION	CC 425
COURSE WEBSITE	Moodle CHEM 495 2222
Strongly recommended TEXTBOOKS	J.M. Hollas, <i>Modern Spectroscopy</i> , 4th ed., Wiley, 2004 D.C. Harris, M.D. Bertolucci, <i>Symmetry and Spectroscopy</i> , Dover, 1989 (reprint from OUP, 1978)
OFFICE HOURS	Mo 14:30-15:30; drop-in “anytime”: just ask if I am available; or email

LECTURES AND READING

Lectures will be delivered in-person, flipped-classroom: voice-over PowerPoint slides are made available as videos on Moodle, for you to view *before* the in-person class. In-class time will be used for your questions, additional explanations or practice problems.

There is no single required textbook for this advanced course, but (parts of) Hollas and Harris are strongly recommended reading. Further “reading” suggestions are provided on Moodle and consist of online links, videos or pdf files. The lectures are designed to convey the wealth of information in a, hopefully, digestible manner that is not overly mathematical.

COURSE OBJECTIVES

- To provide students with a working knowledge of group theory.
- To instruct students in the use of character tables in spectroscopy.
- To develop in students an awareness for spectral features and their information content.

COURSE OUTLINE

- Chapter 1 Molecular symmetry and character tables
- Chapter 2 Electronic spectroscopy
- Chapter 3 Vibrational spectroscopy
- Chapter 4 Rotational spectroscopy

A detailed description with key words covered and links to the lecture videos and slides can be found on Moodle. The pdf slides are for you to print and annotate, before and during the live lecture time. A detailed, by lecture, schedule is also posted.

END-OF-LECTURE QUESTIONS

Every lecture will terminate with one or two questions (on Moodle) that are designed to help you think about the material. They are neither timed nor marked but should be attempted as soon as possible after each lecture. Details on the end-of-lecture questions can be found on Moodle.

PROBLEM SETS/ACTIVITIES

There will not be formal problem sets or assignments. However, selected problems to solve for practice and their answers are posted on Moodle. You should work through the problems after the topic is addressed in class and pay particular attention to how the information is given in the answers.

QUIZZES

There will be four (4) formal evaluations, during lecture time and in-person in class, tentatively scheduled for

September 28, 2022: Molecular Symmetry;

October 26, 2022: Electronic Spectroscopy;

November 16, 2022: Vibrational Spectroscopy;

December 2, 2022: Rotational Spectroscopy.

All quizzes are “open book”: your class notes and character tables are allowed, in printed form or electronically.

If you are absent from a quiz, you must present 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 Professor as soon as possible but **no later than one (1) week after the quiz**. The Department determines the validity of the absence. A make-up quiz will **only** be offered if the absence is valid. If the excuse is absent or not valid, a mark of zero will be awarded for your quiz.

ACADEMIC HONESTY (*Source: <http://www.concordia.ca/students/academic-integrity.html>*)

Go to the link above and familiarize yourself with what you are supposed to do and what you are supposed to avoid doing. **In short:** maintain your academic honesty at all times! And if you have specific questions on this, ask.

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.”

Clarifications: “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 whose phrasing still closely resembles that of the original source. It could be the work of a fellow student, e.g., a problem set completed by another student, or unauthorized data for a presentation. 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.

In these “**internet times**”, the following are also offenses:

- for **lectures and related material**: unauthorized recordings; distribution of such material (electronically or otherwise);
- for **evaluative exercises**: use of any unauthorized material; making copies (through scans, photos, videos...) of the evaluation material, and distribution of such material.

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 to the Dean's office.

“CHEM 101”

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 2017 or more recently)**, you have fulfilled the requirement. You are exempt, if you can locate your ID, with no

associated entry, in the pdf file located on the Departmental web site (<http://www.concordia.ca/content/dam/artsci/chemistry/docs/compliance-list.pdf>).

The aim of the seminar and quiz is to clarify which academic practices are considered unacceptable by the Department of Chemistry and Biochemistry. The seminar will be offered during the third week of classes (see the appendix for the dates and times offered); the quiz is online, can be accessed through the MyConcordia portal (on Moodle, choose CHEM 101 under Specialized Chemistry Sites) 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.

COURSE GRADE

The final grade of the course is composed as follows:

Quizzes (4) 100% (25% each)

The minimum passing mark is 50% (D-).

Grading scale (percentage to letter grade; normal rounding applies):

Passing Grades:

A+	A	A-	B+	B	B-	C+	C	C-	D+	D	D-
100-90	89-85	84-80	79-77	76-73	72-70	69-67	66-63	62-60	59-57	56-53	52-50

Failing Grade:

F
<50

In the event of extraordinary circumstances beyond the University's control (by now, we all know what that potentially means!), the content and/or evaluation scheme in this course is subject to change. Let's all hope we won't need to invoke this clause.

H.M. Muchall, July 2022

Appendix

Seminar on academic conduct

Date (Fall 2022)	Time	Mode	Registration link
Sept. 21 (Wednesday)	21:00-22:00	Zoom	https://concordia-ca.zoom.us/meeting/register/tZYkduivqDkpHtVmJllg74uA5HiKQC-ZaM8
Sept. 22 (Thursday)	21:00-22:00	Zoom	https://concordia-ca.zoom.us/meeting/register/tZElc-6rrzwvE9WHVZfXXuhROaPhEUnVARTU
Sept. 26 (Monday)	19:00-20:00	Zoom	https://concordia-ca.zoom.us/meeting/register/tZAsc-iqqzkrGNIX7oPpwXcdqVH9Mc3inWP8

As space for each of the Zoom seminars is limited, please **register** early for your preferred evening slot (copy the corresponding link above into your browser, and make sure you do not introduce a space: it is "concordia-ca"). Then do not forget to **attend** that seminar slot on the corresponding date. We will take attendance at the Zoom seminar.