

UNIVERSITY OF TORONTO
DEPARTMENT OF CHEMISTRY

CHM441F/CHM1005F

Spectroscopic Analysis in Organic Chemistry

Fall 2020

COURSE DESCRIPTION

This course will discuss the application of spectroscopic methods available to graduate students and researchers, including IR, ^1H NMR, ^{13}C NMR, and MS. Emphasis will be upon the practical aspects of each method and students will learn how to interpret data to elucidate the structure of complex organic molecules.

OUTLINE OF COURSE CONTENT

1. Elemental Analysis and Mass Spectrometry. Elemental analysis and empirical formula. Mass spectrometry techniques and interpretation.
2. Infrared Spectroscopy. Vibrational spectroscopy principles. Characteristic IR frequencies of organic functional groups.
3. NMR spectroscopy I. The NMR experiment. ^1H , ^{13}C and heteronuclear NMR spectroscopy. Coupling constant analysis. Case studies.
4. NMR spectroscopy II. Advanced NMR spectroscopy. Second order coupling, quadrupolar nuclei and two-dimensional NMR experiments. Case studies.

STUDENT LEARNING OUTCOMES

By the end of the course, students should be able to:

1. explain the important principles and practices upon which the techniques of mass spectrometry, elemental analysis, and IR and NMR spectroscopy are based;
2. critically ascertain the appropriate spectroscopic technique(s) to be used in the determination of any organic structure;
3. interpret spectroscopic data to fully elucidate the structure of complex organic molecules;
4. apply their theoretical and practical knowledge in lab exercises comparing calculated spectra with experimental spectra and fully characterizing the structure of an unknown organic molecule.

INSTRUCTORS

Prof. Barb Morra (lecture: Sept. 10 – Oct. 6 EDT)

barb.morra@utoronto.ca

Office Hours: Thursdays 11:00 am – 12:00 pm Eastern Time (ET) or by appointment

Prof. Scott Browning (lecture: Oct. 8 – Dec. 8 EDT/EST)

cs.browning@utoronto.ca

Office Hours: Thursdays 11:00 am – 12:00 pm Eastern Time (ET) or by appointment

Mr. Rick Fu (laboratory: Wednesdays, 10:00 a.m. – 1:00 p.m. Eastern Time (ET) (October – November))

rick.fu@mail.utoronto.ca

COURSE INFORMATION

Class Meetings

In this fully online course, there is no in-person scheduled classroom time. Each week, synchronous class meetings will take place with the course instructors via BB Collaborate at the times shown below. You are expected to attend these class meetings. Synchronous class meetings with the lab instructor will take place beginning in mid-October. Class meetings may not be reproduced, posted or shared. Recordings of class meetings will be provided to students who require them on the basis of academic accommodations.

Synchronous Class Times

Lecture: Tuesdays and Thursdays, 10:00 – 11:00 a.m. ET

Laboratory: Wednesdays, 10:00 a.m. – 1:00 p.m. ET (October – November)

Expectations regarding online etiquette

The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. U of T does not condone discrimination or harassment against any persons or communities.

Course Website

Important information including course lecture notes, laboratory information and assessment information will be posted on the CHM441H/1005H course website on Quercus (<https://q.utoronto.ca>). Please check the course website regularly for announcements and postings.

Course Materials

Optional Textbooks: Pavia *et al*, *Introduction to Spectroscopy*, 5th Ed., Cengage, 2015

Silverstein *et al*, *Spectrometric Identification of Organic Compounds*, 8th Ed., Wiley, 2015

Articles from the primary research literature may also be posted on the course website throughout the semester.

Tests and Assignments

Tests and assignments will be provided during the term as documents in PDF format to be downloaded from the course website. Completed tests and assignments must be sent via email as a PDF to the appropriate instructor by the allotted deadline. Assignments are expected to be completed electronically while the midterm test and final examination are expected to be hand-written by traditional (paper and pen) or electronic (tablet and stylus pen) methods.

Marking Scheme

Please pay careful attention to the due dates and times for each course component.

<i>Course Components</i>	<i>Weight</i>	<i>Dates</i>
Assignments (2)	10%	<i>Due:</i> 10:00 am on Tues. October 13 10:00 am on Thurs. November 26
Computation Laboratory	10%	<i>Lab:</i> Wed. October 14; <i>Due:</i> 10:00 am on Tues. October 27
Term Test	25%	Tues. October 20, 10:00 – 11:00 am
Unknown Cmpd Laboratory	20%	<i>Lab:</i> Wed. October 28; <i>Due:</i> 10:00 am on Thurs. November 26
Final Assignment	35%	TBA

Note: All assignments and laboratory reports will be submitted as electronic copies by the stipulated deadlines. The final assignment will be written during the Faculty of Arts & Science December final assignment period. Late work will be accepted with a deduction of 10% per day for a maximum of 4 days. Completed assignments will not be accepted once marked work has been returned to students.

Technology Requirements

This course requires the use of computers, and of course sometimes things can go wrong when using them. You are responsible for ensuring that you maintain regular backup copies of your files, use antivirus software (if using your own computer), and schedule enough time when completing an assignment to allow for delays due to technical difficulties. Computer viruses, crashed hard drives, broken printers, lost or corrupted files, incompatible file formats, and similar mishaps are common issues when using technology, and are not acceptable grounds for a deadline extension.

Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here: <https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/> . Advice for students more broadly regarding online learning is available here: <https://onlinelearning.utoronto.ca/getting-ready-for-online/>

E-mail Policy

When sending an e-mail, please include the course code CHM441/1005 in the subject line and use your UTOR e-mail account only. You will normally receive a response within 48 hours. Please keep in mind that lengthy explanations of course material are best discussed during office hours. Please do not send emails through Quercus.

Privacy Policy

This course, including your participation, will be recorded on video. Course videos and materials belong to your instructor, the University, and/or other sources and are protected by copyright. Do not download, copy, or share any course or student materials or videos without the explicit permission of the instructor.

Academic Integrity

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters (<https://governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019>) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In papers and assignments:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Submitting your own work in more than one course without the permission of the instructor.
3. Making up sources or facts.
4. Obtaining or providing unauthorized assistance on any assignment.

On tests and exams:

1. Using or possessing unauthorized aids.
2. Looking at someone else's answers during an exam or test.
3. Misrepresenting your identity.

In academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see <https://www.academicintegrity.utoronto.ca/>).

Accessibility

The University of Toronto is committed to accessibility. If you require accommodations for a disability, or have any accessibility concerns about the course, the classroom or course materials, please contact Accessibility Services as soon as possible:

disability.services@utoronto.ca or <https://studentlife.utoronto.ca/department/accessibility-services/>