Fall 2020

CHEM 702-101: Special Topics: Spectrometric Identification of Organic Compounds

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NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Fall 2020 Course Syllabus

CHEM 702 – Special Topics: Spectrometric Identification of Organic Compounds

NJIT Academic Integrity Code: The shift to remote and converged teaching due to the COVID-19 pandemic has required that both instructors and students make changes to their normal working protocols for courses. Students are asked to practice extra care and attention concerning academic honesty, with the understanding that all cases of plagiarism, cheating, multiple submission, and unauthorized collaboration are subject to penalty. Students must properly cite and attribute all sources used for papers and assignments. Students may not collaborate on exams or assignments, directly or through virtual consultation, unless the Instructor gives specific permission to do so. Posting an exam, assignment, or answers to them on an online forum (before, during, or after the due date), in addition to consulting posted materials, constitutes a violation of the university's Honesty policy. Likewise, unauthorized use of live assistance websites, including seeking "expert" help for specific questions during an exam, can be construed as a violation of the honesty policy. All students should be familiar with the NJIT Academic Integrity Code.

All Students should be aware that the Department of Chemistry & Environmental Science (CES) takes the **NJIT Academic Integrity Code** very seriously and enforces it strictly. This means that there must not be any forms of plagiarism, i.e., copying of homework, class projects, or lab assignments, or any form of cheating in quizzes and exams. Under the University Code on Academic Integrity, students are obligated to report any such activities to the Instructor.

COURSE INFORMATION

Course Description: Spectroscopic methods for structure analysis focused on Nuclear Magnetic Resonance Spectrometry (NMR). Other techniques such as Mass Spectrometry (MS), Infrared/Raman (IR/Raman)), and Ultraviolet-Visible (UV-VIS) Spectroscopies will be covered as complementary analytical techniques. Fundamentals of the NMR phenomenon, the relationship between NMR spectra and molecular structure. Recording of routine spectra (^{1}H and ^{13}C), essentials of data processing (e.g., weighting functions). 1D NMR techniques: Decoupling, DEPT, relaxation measurement, magnetization transfer, NOE difference spectra. 2D NMR techniques: Homo- and heteronuclear correlation (COSY, TOCSY, HSQC, HMBC), measurement of the nuclear Overhauser effect (NOESY, ROESY). Emphasis is on learning the practical use of the NMR instrument.

Number of Credits: 3

Prerequisites: Knowledge of organic chemistry and basic laboratory techniques.

Course-Section and Instructor

Course-Section	Instructor
Fall 2020-Chem 702-101	Carlos Pacheco, Ph.D. carlos.n.pacheco@njit.edu
	Email: carlos.n.pacheco@njit.edu
	Office: B006; NMR laboratory: B008

Class time: M, 6 PM - 8:50 PM
Office Hours: 1) **IN-PERSON**, by appointment, one-by-one, 30-min: Thursdays, 11 am-12 pm;
2) **VIRTUAL, WebEx**, GROUP meeting: Thurs, 12 pm-12:30 pm.
Email: All emails should include **CHEM702** in the subject so that it can be filtered appropriately.

Textbook:

Title	*Spectrometric Identification of Organic Compounds*
Author	Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce
Edition	8th
Publisher	John Wiley & Sons
ISBN #	978-0-470-61637-6

University-wide Withdrawal Date: The last day to withdraw with a W is Monday, November 9, 2020. It will be strictly enforced.

Learning Outcomes:

1. Use NMR spectrometers.
2. Identify organic compounds by analysis and interpretation of spectral data.
3. Explain common terms in NMR spectroscopy such as chemical shift, coupling constant, and anisotropy and describe how they are affected by molecular structure.
4. Analyze and interpret 1D and 2D NMR spectra.
5. Acquire the ability to investigate and determine the structure of typical organic chemical compounds (molecular weight up to ca. 500 Da) using suitable NMR experiments.
6. Perform the most commonly used NMR experiments, and to interpret and document their results.
7. Concepts of Mass Spectrometry (MS), and Infrared/Raman (IR, Raman) and Ultraviolet-Visible (UV-VIS) Spectroscopies.

POLICIES

All CES students must familiarize themselves with, and adhere to, all official university-wide student policies. CES takes these policies very seriously and enforces them strictly.

SAFETY:

Observation and use of an NMR instrument require following a critical set of safety procedures and guidelines (it may be found here). Students are advised that they will be asked to read and accept safety procedures and guidelines before participation in the class is confirmed.

Grading Policy: The final grade in this course will be determined as follows:

Homework/Quizzes	10%
Midterm Exam I	20%
Midterm Exam II	20%
Presentations of Spectroscopic Data	20%
Final	30%

Your final letter grade in this course will be based on the following tentative grading scale:

A	90%	C	70%
B+	85%	D	60%
B	80%	F	<60%
C+	75%		

Attendance Policy: Attendance at classes will be recorded and is mandatory. Each class is a learning experience that cannot be replicated through merely "getting the notes."

Homework Policy: Homework is an expectation of the course. The homework problems set by the Instructor are to be handed in for grading and will be used in the determination of the final letter grade as described above.

Exams: There will be two midterm exams during the semester and one comprehensive final exam. The following exam periods are tentative and therefore, possibly subject to change:

Midterm Exam I	10/12
Midterm Exam II	11/23
Final Exam Period	December 15 - 21, 2020

The final exam will test your knowledge of all the course material taught in the entire course.

Makeup Exam Policy: There will typically be **NO MAKEUP QUIZZES OR EXAMS** during the semester. If a student has a legitimate reason for missing a quiz or exam, the student should contact the Dean of Students' office. The student should present a written, valid proof of the reason for missing the exam, e.g., a doctor's note, police report, court notice, etc. clearly stating the date AND time of the mitigating problem. The student must also notify the CES Department Office/Instructor that the exam will be missed so that appropriate steps can be taken to make up the grade.

Cellular Phones: All mobile phones and other electronic devices must be switched off during all class times. Such devices must be stowed in bags during exams or quizzes.

ADDITIONAL RESOURCES

Accommodation of Disabilities: Office of Accessibility Resources and Services (formerly known as Disability Support Services) offers long term and temporary accommodations for undergraduate, graduate, and visiting students at NJIT.

If you need accommodations due to a disability, please contact Chantonette Lyles, Associate Director at the Office of Accessibility Resources and Services at 973-596-5417, or via email at lyles@njit.edu. The office is located in Fenster Hall Room 260. A Letter of Accommodation Eligibility from the Office of Accessibility Resources Services office authorizing your accommodations will be required.

Date	Day	Event
September 1	T	First Day of Classes
September 8	T	Last Day to Add/Drop Classes
November 9	M	Last Day to Withdraw
November 25	W	Friday Classes Meet
November 28 – November 29	R - Su	Thanksgiving Break - University Closed
December 10	R	Last Day of Classes
December 11	F	Reading Day 1
December 14	M	Reading Day 2
December 15-21	T-M	Final Exam Period

For further information regarding self-identification, the submission of medical documentation and additional support services provided, please visit the Accessibility Resources and Services (OARS) website at http://www5.njit.edu/studentsuccess/disability-support -services/

Important Dates (See: Fall 2020 Academic Calendar, Registrar)

Class Participation - Class participation includes, but is not limited to, class engagement, attendance, and response to questions during class. It is a discussion-driven and student-centered course, students are expected to be actively involved in discussions and other class activities that would generate the robust energy needed for a fruitful conversation. Active participation includes completing assignments on time, being present for impromptu class discussions and quizzes. Students who record four or more unexcused absences will receive no points for class participation. You are strongly advised to use all means available to contact me if you need to be excused from class in an emergency. When you miss a class, it will be your responsibility to find out what was discussed.

Literature Research/Group Learning - Group learning is a prospective approach to be pursued as part of this course. The objective is to instill creative-problem solving skills and to relate the concepts of chemistry principles to real-life situations. Students will be grouped into sub-teams, and each team is required to diagnose these problems in a team setting during class and provide answers. A typical problem-solving class exercise will require analytical, evaluative, or creative thinking. Students would need to explain familiar phenomena in terms of course concepts.

Course Outline

Lecture	Section	Topic	Assignment
1	9/8	Introduction to NMR	video
2	9/14	^{1}H: Chemical Shift, Couplings, spectra interpretation	Reading: Chapter 3.1 to 3.7
3	9/21	^{1}H: Chemical Equivalence, Magnetic Equivalence, Chirality, case studies	Reading: Chapter 3.8 to 3.16
4	9/28	^{13}C: Chemical Shift, Couplings, spectra interpretation	Reading: Chapter 4
5	10/5	^{13}C: ^{1}H Decoupling, Nuclear Overhauser Effect, Polarization Transfer, DEPT, INEPT, APT	Reading: Chapter 4
6	10/12	Multinuclear NMR (nuclei other than ^{1}H and ^{13}C) **Midterm Exam I**	Reading: Chapter 6
7	10/19	Practical NMR -- in the lab (1D NMR)	Operational Guide
8	10/26	2D NMR: through-bond correlation Spectroscopy - **homononuclear** shift correlation- COSY, TOCSY, INADEQUATE	Reading: Chapter 5.1 to 5.3; 5.4.1; 5.5.1; 5.6; 5.7.1, 5.8
9	11/02	2D NMR: through-space correlation Spectroscopy, NOESY, ROESY	Reading: Chapter 5.10
10	11/09	2D NMR: **Heterononuclear** shift correlation – HSQC, HMBC	Reading: Chapter 5.4.2 to 5.4.5; 5.5.2 to 5.5.3; 5.7.2 to 5.7.3.
11	11/16	Practical NMR -- in the lab (2D NMR)	Operational Guide
12	11/23	Infrared Spectroscopy (IR), Raman; Mass Spectrometry (MS) **Midterm Exam II (take home)**	Reading: Chapters 1 and 2
13	11/30	Mass Spectrometry (MS)	Reading: Chapter 1
14	12/7	Students Presentations of Spectroscopic Data	

Updated by Carlos Pacheco – August 2020
Department of Chemistry & Environmental Sciences (CES)
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