Fall 2021

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 2021 Course Syllabus

CHEM 702-101 – 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 both instructors and students to change their standard working protocols for courses. Students are asked to practice extra care and attention concerning academic honesty, 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. 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 violating 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 structural analysis concentrated on Nuclear Magnetic Resonance Spectroscopy (NMR). Other techniques such as Mass Spectrometry (MS), Infrared/Raman (FTIR, Raman), and Ultraviolet-Visible (UV-VIS) are covered as supplementary analytical techniques. Fundamentals of the NMR phenomenon, relationship of NMR spectra to molecular structure. Recording of routine spectra (1H and 13C), essential components of data processing (e.g., weighting functions). 1D-NMR techniques: Decoupling, DEPT, Relaxation measurements, magnetization transfer (INEPT), NOE difference spectra, selective experiments (NOESY-1D, ROESY-1D). 2D-NMR techniques: Homo- and Heteronuclear correlation (COSY, TOCSY, HSQC, HMBC), the use of nuclear Overhauser effect (nOe) through NOESY and ROESY to establish the stereochemistry of the molecule. One of the main goals is to learn the hands-on use of NMR instruments. The simultaneous output of the course is a robust interpretation of spectroscopic data to achieve plausible structures.

Number of Credits: 3
Prerequisites: Knowledge of organic chemistry and basic laboratory techniques.

Course-Section and Instructor

Course-Section	Instructor
Fall 2021-Chem 702-101	Carlos Pacheco, Ph.D.
	Email: carlos.n.pacheco@njit.edu
	Office: B006; NMR laboratory: B008

Class time: Mondays, 6 PM - 8:50 PM
Office Hours: Thursdays, 11 AM-12 PM
Email: All emails should include **CHEM702-101:** in the subject so that it can be appropriately sorted.
Delivery of instruction: Convergent (or Hybrid): Some traditional face-to-face contact hours are replaced with required synchronous (or asynchronous) online instruction (frequently through the learning management system - LMS). Students should refer to the course syllabus for the course meeting schedule. However, **no hybrid course should be more than 50% online**.

Textbook:

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

University-wide Withdrawal Date: The last day to withdraw with a W is Friday, November 10, 2021. It is strictly enforced.

Learning Outcomes:
1. Use NMR spectrometers.
2. Identify organic compounds by analysis and interpretation of spectral data.
3. Explain standard 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 typical organic chemical compounds (molecular weight up to *ca.* 500 Da) using suitable NMR experiments.
6. Perform the most used NMR experiments and interpret and document their results.
7. Concepts of Mass Spectrometry (MS), and Infrared/Raman (FTIR, 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 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%
Presentation(s)	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 is recorded and mandatory. Each class is a learning experience that cannot be replicated by 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 to determine the final letter grade as described above.

Exams: There are wo 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	10/11
Midterm Exam II	11/22
Final Exam Period	December 15 - 21, 2021

The final exam tests 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 Student's Office. The student should present written, valid proof of the reason for missing the exam, *e.g.*, a doctor's note, police report, or court notice, 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, don't hesitate to contact Chantonette Lyles, Associate Director at the Office of Accessibility Resources and Services, at 973-596-5417 or 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 authorizing your accommodations is required. 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 2021 Academic Calendar, Registrar)

Date	Day	Event
September 1	W	First Day of Classes
September 8	W	Monday Classes Meet
September 8	W	Last Day to Add/Drop Classes
November 10	W	Last Day to Withdraw from Classes
November 25 – November 28	R - Su	Thanksgiving Break - University Closed
December 10	F	Last Day of Classes
December 13	M	Reading Day 1
December 14	T	Reading Day 2
December 15-21	W-T	Final Exam Period

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 to 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 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 is 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 relate the concepts of chemistry principles to real-life situations. Students group into 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 requires 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	9/13	^{1}H: Chemical Shift, Couplings, spectra interpretation	Reading: Chapter 3.1 to 3.7
3	9/20	^{1}H: Chemical Equivalence, Magnetic Equivalence, Chirality, case studies	Reading: Chapter 3.8 to 3.16
4	9/27	^{13}C: Chemical Shift, Couplings, spectra interpretation	Reading: Chapter 4
5	10/4	^{13}C: ^{1}H Decoupling, Nuclear Overhauser Effect, Polarization Transfer, DEPT, INEPT, APT	Reading: Chapter 4
6	10/11	Multinuclear NMR (nuclei other than ^{1}H and ^{13}C) **Midterm Exam I**	Reading: Chapter 6
7	10/18	Practical NMR -- in the lab (1D NMR)	Operational Guide
8	10/25	2D NMR: through-bond correlation Spectroscopy - **Homononuclear** shift correlation- COSY, TOCSY, INADEQUATE 2D NMR: through-space correlation Spectroscopy, NOESY, ROESY	Reading: Chapter 5.1 to 5.3; 5.4.1; 5.5.1; 5.6; 5.7.1, 5.8 Reading: Chapter 5.10
9	11/01	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.
10	11/08	Advanced topics in NMR	*Guest Speaker:* ***Dr. Gary Martin*** *(co-editor-in-chief of Magnetic Resonance in Chemistry)*
11	11/15	Infrared Spectroscopy (IR), Raman	Reading: Chapter 2, video
12	11/22	UV-VIS **Midterm Exam II (take home)**	Reading material will be uploaded onto CANVAS
13	11/29	Mass Spectrometry (MS)	Reading: Chapter 1
14	12/06	Mass Spectrometry (MS)	Reading: Chapter 1