NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Fall 2024 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 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 directly or through virtual consultation on exams or projects unless the instructor gives specific permission. In addition to consulting posted materials, posting an exam, assignment, or answers to them on an online forum (before, during, or after the due date) 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 know that the Department of Chemistry & Environmental Science (CES) takes the NJIT Academic Integrity Code seriously and strictly enforces it. This means there must be no plagiarism, i.e., copying homework, class projects, lab assignments, or cheating in quizzes and exams. Under the University Code on Academic Integrity, students must report 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 routine spectra (1H and 13C) and essential data processing components (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 methods: 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 2023-CHEM702-101	Carlos Pacheco, Ph.D.
FMH 307; Mondays, 6 PM - 8:50 PM	Email: carlos.n.pacheco@njit.edu
Office Hours: Mondays, 4 PM-6 PM **Virtual: https://njit.webex.com/meet/pacheconjit.edu	Office: B006; NMR laboratory: B008

Email: All emails should include **CHEM702-101:** in the subject so they can be appropriately sorted. **Delivery of instruction**: face-to-face.

Textbooks

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

Title	Spectroscopic Methods in Organic Chemistry
Author	Stefan Bienz, Laurent Bigler, Thomas Fox, Herbert Meier
Edition	3rd
Publisher	Thieme Chemistry
ISBN #	978-3132434080

University-wide Withdrawal Date: The last day to withdraw with Monday, November 11, 2024; 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), 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 policies before participating in the class is confirmed.

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

Homework/Quizzes	20%
Midterm Exam	30%
Presentation(s)	20%
Final	30%

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

A	90-100%	C	70-74.5%
B+	85-89.5%	D	60-69.5%
B	80-84.5%	F	<60%
C+	75-79.5%		

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 will be handed in for grading and used to determine the final letter grade as described above.

Exams: One midterm exam during the semester and one comprehensive final exam. The following exam periods are tentative and, therefore, possibly subject to change:

Midterm Exam	**October 21, 2024**
Final Exam Period	**December 15 - 21, 2024**

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.

Using mobile phones and AI tools responsibly in class to improve the learning experience is crucial. However, it is necessary to keep these devices in bags during exams or quizzes. Also, the use of AI tools is encouraged as learning new technologies is necessary for professional development.

ADDITIONAL RESOURCES

Accommodation of Disabilities: Office of Accessibility Resources and Services (formerly 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 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 https://www.njit.edu/accessibility/.

Important Dates (See: Fall 2024 Academic Calendar, Registrar)

Class Participation - In this course, participation is crucial and involves engaging in discussions, attending classes, and responding to questions. The learning approach is discussion-based and centered around students. To have a productive conversation, active participation is required, which includes completing assignments on time and being present for class discussions and quizzes. Recording four or more unexcused absences results in zero points for class participation. In case of an emergency, it is recommended to contact me through all available means if you need to miss class. It is important to catch up on what was discussed in any missed classes.

Literature Research/Group Learning - As part of this course, we will explore the benefits of group learning. The aim is to develop creative problem-solving skills and link chemistry principles to real-life scenarios. Students will be divided into teams and work together to diagnose problems during class, providing solutions as a group. These exercises will require analytical, evaluative, and creative thinking. Students will also be expected to explain familiar phenomena using the course concepts.

Course Outline

Lecture	Section	Topic	Assignment
1	9/09	Introduction to NMR ^{1}H: Chemical Shift, Couplings, spectra interpretation	Reading: Silverstein - Chapter 3.1 to 3.7
2	9/16	^{1}H: Chemical Equivalence, Magnetic Equivalence, Chirality, case studies	**Quiz 1** Reading: Silverstein - Chapter 3.8 to 3.16
3	9/23	^{13}C: Chemical Shift, Couplings, spectra interpretation	**Quiz 2** Reading: Silverstein - Chapter 4
4	9/30	^{13}C: ^{1}H Decoupling, Nuclear Overhauser Effect, Polarization Transfer, DEPT, INEPT, APT	**Quiz 3** Reading: Silverstein -Chapter 4
5	10/7	Multinuclear NMR (nuclei other than ^{1}H and ^{13}C)	**Quiz 4** Reading: Silverstein - Chapter 6
6	10/14	**Practical NMR -- in the lab (1D NMR)**	**Quiz 5** Reading: Operational Guide, material under https://research.njit.edu/nmrl/training
7	10/21	**MIDTERM**	
8	10/28	2D NMR: through-bond correlation Spectroscopy - **Homonuclear** shift correlation- COSY, TOCSY, INADEQUATE; 2D NMR: through-space correlation Spectroscopy, NOESY, ROESY	**Quiz 6** Reading: Silverstein - Chapter 5.1 to 5.3. 5.4.1; 5.5.1; 5.6; 5.7.1, 5.8 Reading: Chapter 5.10
9	11/04	2D NMR: **Heteronuclear** shift correlation – HSQC, HMBC	**Quiz 7** Reading: Silverstein - Chapter 5.4.2 to 5.4.5; 5.5.2 to 5.5.3; 5.7.2 to 5.7.3.
10	11/11	Infrared Spectroscopy (IR), Raman **Practical NMR -- in the lab (2D NMR)**	**Quiz 8** Reading: Silverstein - Chapter 2, video Stefan Bienz - Chapter 2
11	11/18	Infrared Spectroscopy (IR), Raman **(cont.)** UV-VIS	Reading: Silverstein -Chapter 2, UV-VIS material uploaded on CANVAS Stefan Bienz - Chapter 1
12	11/25	Mass Spectrometry (MS)	**Quiz 9** Reading: Silverstein - Chapter 1. Stefan Bienz – Chapter 4.
13	12/02	Mass Spectrometry (MS)	**Quiz 10** Reading: Silverstein - Chapter 1. Stefan Bienz – Chapter 4.
14	12/09	Presentations of acquired NMR data (1D and 2D)	

Updated by Carlos Pacheco – August 2024
Department of Chemistry & Environmental Sciences
(CES) **Course Syllabus, Fall 2024**