

CHEM 541 / CHEM 364 Organic Chemistry I
Spectral Analysis of Organic Compounds
Course Syllabus - 2013

Course Description: This course provides a working background for the identification of organic compounds encountered in nature, industry, and the research laboratory. An integrated approach to identification is stressed. The major types of spectral data come from mass spectra, infrared spectra, ^1H NMR spectra, ^{13}C NMR spectra, and NMR spectra of several other nuclei. How to interpret these data will be discussed at length with ample problems, some worked in class, to illustrate the techniques. Lecture material will be identical for CHEM 541 and CHEM 364. Exams for CHEM 541 will have some additional questions that are not given on the CHEM 364 exams.

Course Objectives: After completing this course, you should be able to examine spectra for most unknown organic chemicals and be able to determine chemical structures. Specific course goals include:

1. Learn how to use IR spectra to determine functional groups.
2. Learn how to use MS to determine molecular weight.
3. Learn rudiments of ion fragmentation in the mass spectrum.
4. Become familiar with simple ^1H NMR and common proton coupling patterns.
5. Become familiar with ^{13}C NMR spectra including DEPT spectra.
6. Learn simple capabilities of 2D NMR techniques including such as HMQC.
7. Learn how to determine interatomic distance from NOE spectra.
8. Become aware of NMR techniques for less common nuclei such as ^{31}P .

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Required textbook: "Spectrometric Identification of Organic Compounds", 7th edition, Silverstein, Webster and Kiemle, Wiley & Sons: New York, 2005.

Grading: Will be on the basis of 250 pts divided as follows:

assigned problems (50 pts) approximately 5 problem sets will be collected and graded for apparent effort on the part of the student. Photocopy your problems before submission: correct answers will be provided for you at the time of submission. Late problem assignments will be penalized 1/2 of total grade per week.

midterm exam (100 pts) will cover MS, IR and (time permitting) simple NMR

Final Exam (100 pts) will emphasize advanced NMR concepts but will include some IR.

Office Hours: Wednesday 7:30 – 8:30 pm in Disque 508.

Method of Presentation: Spectra and information will be presented by computer projection. Lecture screens will be captured and made available through Drexel Learn. At least one problem-working session will be held in the latter classes.

Course Coverage: The following topics will be covered:

I. Mass Spectra

- A. The mass spectrum: low and high resolution
- B. Ion generation techniques: electron impact, chemical ionization, fast atom bombardment, electrospray, etc.
- C. Fragmentation patterns for common chemical classes
- D. Rearrangements
- E. Molecular formula determination

II. Infrared

- A. Basic principles of IR pertinent to structure identification
- B. Functional group determination for common chemical classes
- C. H-bonding considerations

III. ^1H NMR

- A. General theory of FT NMR
- B. Chemical shifts: basic and more advanced considerations
- C. Structure determination strategies: number, location, intensity and splitting of signals
- D. ^1H - ^1H Coupling constants and their importance
- E. Coupling patterns: first order and non-first order
- F. Decoupling techniques (1D experiment)

IV. ^{13}C NMR

- A. Basic principles
- B. Structure determination strategies: number, location, and splitting of signals. Relative signal intensities.
- C. Introduction to FT NMR pulse techniques: modern signal multiplicity Determination (DEPT spectra).

V. Advanced NMR techniques

- A. More FT NMR pulse techniques
- B. 2D Techniques: COSY, HETCOR, HMQC, HMBC, INADEQUATE, TOCSY
- C. NOE experiments

VI. NMR spectra of ^{19}F , ^{31}P , and ^{15}N (direct and indirect detection).

Academic Policies

Plagiarism, cheating, fabrication and other acts of academic misconduct will not be tolerated. For more information, see material in “academic dishonesty” under the “academic policies” tab at the following link:

http://drexel.edu/studentaffairs/community_standards/studentHandbook/

Students with disabilities should see material under the “health and disability services” tab at the following link:

http://drexel.edu/studentaffairs/community_standards/studentHandbook/

If you are registered and wish to drop or withdraw from this course, see the following link:

http://www.drexel.edu/provost/policies/course_drop.asp

The list of topics may be modified after the term begins. If such changes are made, your Instructor will inform you during class.