CHEM 541 Organic Chemistry I
Spectral Analysis of Organic Compounds
Course Syllabus - 2003

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, ^{1}H NMR spectra, and ^{13}C NMR spectra. How to interpret these data will be discussed at length with ample problems, some worked in class, to illustrate the techniques.

Course Objectives: After completing this course, you should be able to examine spectra for virtually any unknown organic chemical and be able to determine its structure.

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Required textbook: "Spectrometric Identification of Organic Compounds", 6th edition, Silverstein & Webster, Wiley & Sons: New York, 1998.

Grading: Will be on the basis of 240 pts divided as follows:
assigned problems (40 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 1/3 of total grade per week.
midterm exam (100 pts) will cover MS, IR and simple NMR
Final Exam (100 pts) will emphasize advanced NMR concepts but will include some IR.

Office Hours: Monday 5:30 – 7:00 in 12-305.

Method of Presentation: Spectra and information will be presented by overhead projection (bring your text for spectra in the book!) and on the blackboard. 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. ^{1}H 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. ^{1}H-^{1}H Coupling constants
- E. Coupling patterns: first order and non-first order
- F. Decoupling techniques

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: signal multiplicity d

V. Advanced NMR techniques
- A. More FT NMR pulse techniques
- B. Correlation Spectroscopy (COSY)
- C. NOE experiments

VI. NMR spectra of ^{19}F, ^{31}P, ^{29}Si, and and ^{15}N (time permitting).