Chemistry 203: Organic Spectroscopy (course code 41010)
Fall 2002,
Lecture: 11-11:50 am, MWF, 122 MSTB
Discussion: 2-2:50 pm, Fri, 114 RH

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Web Site
http://eee.uci.edu/02f/41010

Textbooks

Optional Textbook

Reference Books

Course Outline
Infrared Spectroscopy
Ultraviolet Spectroscopy
Mass Spectrometry
Basic 1H NMR Spectroscopy (1-D FT NMR) 13C NMR Spectroscopy
Advanced NMR Spectroscopy (advanced 1-D and 2-D techniques)

Problem Sets
There will be weekly problem sets due on Fridays at 2:50 pm.

Discussion Sections
Fridays, 2-2:50 pm. 114 RH. Please be prepared to discuss homework problems.
(Note: Discussion will not meet Friday, September 27.)

Exams
Midterm: Friday, November 6, (tentative) Final: Wed., Dec. 11, 10:30 am - 12:30 pm (tentative)

Grading
Midterm, ~35%; Final, ~45%; Problem sets and discussion participation, ~20%.

Teaching Assistants
Michael Chung, 4402 NS 1; 824-2771, dmchung@uci.edu
David Colby, 4403 NS 1; 824-6787, dcolby@uci.edu

Office Hours
Please catch me right after class or any time my office door is open (typically 9 am - 8 pm each day).
**Reading Assignments**
Weekly reading assignments will be posted on the web site and are to be done prior to the class for which they are assigned.

**Homework Assignments and Participation**
Homework will be graded and will, in conjunction with participation in the discussion sections, count for 20% of the course grade. Weekly homework assignments will be posted on the web site and are to be handed in at the discussion section. Completion of the homework assignments is essential to success in this course.

**Attendance**
Attendance of the lecture and discussion sections is mandatory.

**Grades**
Grades will be posted on the class Web site.

**Academic Honesty**
Academic honesty is strictly enforced on exams, homework, and other aspects of this course. Academic dishonesty will result in a failing grade and a letter in the student's file.

**Cell Phones**
Use of cell phones will result in summary execution. Seriously, receipt of calls during class is remarkably disruptive to the instructor and is inconsiderate to all those present. Cell phones must be turned off (neither on tone or on vibrate) during class.

### A Selected List of Topics to be Covered

**General**
- Degrees of unsaturation
- Solving structures from spectra

**Infrared Spectroscopy**
- Theory, instrumentation, sample preparation
- Characteristic peak positions/intensities/shapes for various functional groups (including alkanes, alkenes, arenes, alkynes, alcohols, aldehydes, ketones, esters, acids, amides, amines, ammonium salts, nitro compounds, nitriles)
- Effect of ring size and unsaturation on carbonyl peak position

**UV Spectroscopy**
- Theory, Instrumentation
- Characteristic absorptions of various functional groups
- Calculation of $\lambda_{max}$ for polyenes, unsaturated carbonyl compounds, aromatic carbonyl compounds, other aromatic compounds

**Mass Spectrometry**
- Theory, instrumentation, ionization/vaporization techniques
- High resolution mass spectrometry
- Isotopic abundances, M+1, M+2 peaks
- Fragmentation pathways
- Additional topics TBA

**$^1$H NMR Spectroscopy**
- Theory, instrumentation, sample preparation, peakshape, shimming, digital resolution, etc.
- Chemical shifts (common functional groups, estimation and calculation of chemical shifts)
- Spin-spin coupling (first order spectra, non-first order spectra, virtual coupling, long-range coupling, typical coupling constants)
- Chemical and magnetic equivalence (diastereotopicity, enantiotopicity)
- Pople Notation
- Analysis of spectra as applied to determination of coupling constants and stereochemistry
- Characterization of compounds by $^1$H NMR

**$^{13}$C NMR Spectroscopy**
- Theory, types of simple experiments
- Chemical shifts and substituent effects (common functional groups, estimation and calculation of chemical shifts)
- Spin-spin coupling ($^1$CH, $^2$CH, $^3$CH, $^{13}$C-$^{13}$C coupling, $^{13}$C-$^{19}$F coupling, $^{13}$C-$^{31}$P coupling, typical coupling constants, roles of hybridization, electronegativity, etc.)

"Advanced" $^1$D NMR
- Time-dependent effects (coalescence temperature, $^r$, $^\Delta G^+$, Eyring equation)
- Nuclear Overhauser effect (difference NOE, multi-spin systems, distance-effects, application to stereochemical problems)
- Complex pulse sequences (the rotating frame, effects of various types of pulses, the spin-echo experiments, DEPT)
- $^1$H decoupling experiments
- Additional topics TBA

**2-D NMR**
- 2D J-resolved NMR spectroscopy (theory, heteronuclear, homonuclear, types of 2-D plots, geminal coupling, vicinal coupling, allylic coupling, long-range coupling)
- COSY (interpretation, digital resolution, contour levels)
- HETCOR (H,C-COSY) and HMQC
- Long-range H,C-COSY (HETCOR) and HMBC
- TOCSY
- INADEQUATE
- NOESY
- ROESY
- Systematic application of 1-D and 2-D NMR data to the determination of molecular structure
- Additional topics TBA