Organic Spectroscopy
Chem 203, Fall 2020, Course Code 41400

Lecture: 9-9:50 am, MWF,
Discussion: 5-5:50 pm, M

James S. Nowick, 4126 NS 1
949-824-6091, jsnowick@uci.edu,

Web Site
https://canvas.eee.uci.edu/courses/30256
A PDF of the syllabus is available through the course website (Syllabus.pdf).

Textbooks (Required)
• Spectrometric identification of organic compounds. 8th ed.
Robert M. Silverstein, Francis X. Webster, David Kiemle, and David L. Bryce. Wiley, 2014.
NOTE: The 7th edition is also OK.
• Structure determination of organic compounds : tables of spectral data. 4th ed.
E. Pretsch, P. Buhlmann, and M. Badertscher. Springer, 2009.
NOTE: The 3rd edition is also OK.

Additional Items (Required)
• A three-button mouse, such as the Kensington Mouse-in-a-Box or the Microsoft Basic Optical Mouse. This item is required for use in the first discussion section and in subsequent activities and exercises.
• A good ruler, such as the C-Thru model W-30 or model 36 (clear plastic rulers graduated in cm and inches)
• A grid that can be printed laserprinted directly on transparency film is available through the course website (Grid10V2.pdf). This item will be distributed later in the course.
• A laserprinter or good quality inkjet printer, capable of printing homework sets and exams.

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

Problem Sets
There will be weekly problem sets due on Mondays at 5:50 pm.

Discussion Section
5-5:50 pm, Mondays. Please be prepared to discuss homework problems.

Cancelled Classes and Discussion Sections
Class and Discussion Sections will not meet on the scheduled holidays of Wednesday, November 11 and Friday, November 27.

Exams
Midterm: 9 am Saturday, November 14. Part I closed book, 1 hour; Part II open book, open notes, laptop computers permitted, open ended.
Final: 9 am Saturday, December 19. Open book, open notes, laptop computers permitted, open ended.

Grading
Midterm, ~40%; Final, ~45%; Problem sets and discussion participation, ~15%.

Teaching Assistant
James Griffin (jhgriffi@uci.edu), cell phone (###) ###-####. (Set up Zoom calls at any time by appointment.)

Office Hours and Study Sesssion
Fridays at 5-7 pm, or by appointment.
James Griffin (jhgriffi@uci.edu) will be available by appointment.

Sunday Evening Jam Session
There will be a Sunday evening jam session at 5-7 pm every Sunday to go over the homework before it is due that will be hosted by James Griffin. Attendance is optional.

Reading Assignments
Weekly reading assignments will be posted on the Canvas course space as part of each homework assignment and are to be done prior to the due date for that homework assignment.

Homework Assignments and Participation
Homework will be graded and will, in conjunction with participation in the discussion sections, count for 15% of the course grade. Weekly homework assignments will be posted on the Canvas course space and are to be turned in electronically or as a hard copy shortly after each discussion section. Completion of the homework assignments is essential to success in this course.

NOTE: You are permitted to annotate your homework assignments during discussion *using a different sort of pen or pencil*. You will receive some credit for annotated answers if you show appropriate thinking and work. This does not mean that you are allowed to do your homework during discussion section, but rather that you are permitted to correct errors and provided insights on problems on which you have already made good-faith efforts.

Attendance
Attendance of the lecture and discussion sections is mandatory. Please contact me by e-mail at jsnowick@uci.edu if you are unable to attend, and I will make accommodations. I am requesting that you please keep your cameras on during lecture and discussion sections, as I very much want this to be like a normal class, and I just can't lecture to an empty room.
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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. NOTE THAT USE OF SOLVED HOMEWORK SETS AND ANSWER KEYS FROM PREVIOUS YEARS' CLASSES IS NOT PERMITTED AND CONSTITUTES ACADEMIC DISHONESTY.

While it is OK to discuss problems with your classmates, it is NOT OK to simply copy the answers of your classmates.

Accommodations for the COVID-19 Pandemic
Accommodations for will be made liberally by Professor Nowick. Please contact me by e-mail at jsnowick@uci.edu if you have any special needs. Printed copies of all homework assignments and exams will be made available upon request. Please contact TA James Griffin at jhgriffi@uci.edu to arrange for copies to be made and picked up. Lectures and Discussion sections will be recorded on Zoom and made available.

A Selected List of Topics to be Covered

General

Degrees of unsaturation
Molecular modeling and conformational analysis
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

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
Additional topics TBA

^{13}C NMR Spectroscopy

Theory, types of simple experiments (^{1}H decoupling, off-resonance ^{1}H decoupling, DEPT, APT)
Chemical shifts and substituent effects (common functional groups, estimation and calculation of chemical shifts)
Spin-spin coupling ($^{1}J_{CH}$, $^{2}J_{CH}$, $^{3}J_{CH}$, ^{13}C-^{13}C coupling, ^{13}C-^{19}F coupling, ^{13}C-^{31}P coupling, typical coupling constants, roles of hybridization, electronegativity, etc.)
Additional topics TBA

"Advanced" 1-D NMR

Time-dependent effects (coalescence temperature, "τ", $\Delta G^{\ddagger}$, 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, APT, DEPT)
^{1}H decoupling experiments
Additional topics TBA

2-D NMR
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
HMQC-TOCSY
Additional topics TBA