CHEM 647-600: Spectroscopy in Organic Chemistry

Spring 2012 SYLLABUS

T/Th 2:20-3:35 pm, CHAN 2121

PROFESSOR: **Dr. Janet Bluemel**—Reed McDonald building (RMD), room 323 (via 321)
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OFFICE HOURS: **T/Th 3:45-5:00 pm**, or by appointment

TEACHING ASSISTANT: **Eric Steffensmeier—**RMD, room 428 or 402 (both via room 428)
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OFFICE ASSOCIATE: **Jennifer Belcik**—RMD, room 321, only afternoons, 1-5pm
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TEXTBOOKS:

Indispensible:

1. "Organic Structural Spectroscopy", Joseph B. Lambert, Herbert F. Shurvell, David A. Lightner, R. Graham Cooks, Prentice Hall, Upper Saddle River, New Jersey 07458, 2nd Edition 2011, ISBN: 0-13-258690-8

2. "Organic Structure Analysis", Phillip Crews, Jaime Rodriguez, Marcel Jaspars, Oxford University Press, 1st Edition 1998, ISBN: 0-19-510102-2

3. "Organic Structures from Spectra", L. D. Field, S. Sternhell, J. R. Kalman, Wiley & Sons, Ltd, 3rd Edition 2002, ISBN: 0-470-84362-4

Optional:

4. "NMR for Physical and Biological Scientists", Thomas C. Pochapsky, Susan S. Pochapsky, Taylor & Francis, New York, London, 1st Edition 2007, ISBN: 0-8153-4103-2

COURSE GRADING:

Midterm Exam (Tuesday, March 6, 2012, 2:20-3:35 pm, CHAN 2121)	40%
Final Exam (Monday, May 7, 2012, 1:00-3:00 pm, CHAN 2121)	60%

COURSE DESCRIPTION and LEARNING GOALS:

My aim is to provide a comprehensive and contemporary introduction to the diverse and fascinating spectroscopic methods in organic chemistry. All students will be trained in interpreting individual spectra and sets of spectra obtained by different methods, so that molecular compounds and materials are quickly and efficiently characterized with respect to their structure, potential dynamics, and stereochemistry. Special emphasis will be placed on discussing and documenting the data. Recent examples from the literature and seminar talks presented by visitors will be discussed.

COURSE OUTLINE:

I. One-Dimensional NMR Spectroscopy of Liquids

(1) The basics of NMR spectroscopy
- the NMR experiment and the main parts and functions of the NMR spectrometer
- the chemical shift and referencing with internal and external standards
- the J-coupling
- signal assignments and spectrum interpretation
- processing NMR spectra
- T_1 and T_2 relaxation times and more special pulse sequences and tricks

(2) Data documentation and management
- extracting data from spectra and writing them into experimental sections of theses and papers
- archiving data

II. IR Spectroscopy

III. UV/VIS Spectroscopy and Fluorescence

IV. Mass Spectrometry (MS)

V. Two-Dimensional NMR

- standard correlation spectroscopy (homo- and heteronuclear COSY, NOESY etc.)
- special methods (DOSY etc.)

VI. Special Topics

1. NMR Spectroscopy of Solids

(1) Interactions in the solid state
- chemical shift anisotropy
- dipolar interactions
- quadrupolar interactions

(2) Technical requirements of the solids NMR spectrometer
- probeheads for Magic Angle Spinning (MAS)
- high-power decoupling and cross polarization (CP)
- HRMAS of polymers, dendrimers, biomaterials, and surface-bound substances

2. Analytical Methods in Organometallic Chemistry

(1) Multinuclear and organometallic NMR spectroscopy
- common spin-1/2 nuclei, e.g. ^{19}F, ^{31}P, ^{29}Si, ^{119}Sn
- quadrupolar nuclei, e.g. ^{2}H, ^{6}Li, ^{11}B, ^{14}N

(2) NMR of diamagnetic organometallic compounds
- peculiarities of $^{1}H/^{13}C$ chemical shifts
- different J-coupling scenarios and virtual couplings
- dynamic processes and *in situ* reactions

(3) Paramagnetic NMR spectroscopy of organic radicals and organometallic compounds

VII. Most Recent Applications of Liquids and Solids NMR

Besides the textbooks listed above the students will be provided with lecture and exercise materials, and the presented powerpoint slides. All students should have the first three textbooks listed above, because many exercise and problem sets will be taken from them. There will be one written midterm, and one written final exam, which count 40% and 60% of the overall grade. Additionally, there are many homework sets that will not be graded, but discussed. Students are also welcome to bring NMR problems from their own graduate work for discussion, or to give presentations.

Summary: The course 647 will cover IR, UV/VIS, and MS, besides modern one- and two-dimensional NMR techniques for liquids, slurries and solids of small molecular compounds and materials such as polymers.
