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:

Optional:

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
       - T1 and T2 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.  

The Americans with Disabilities Act (ADA) is a federal antidiscrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please contact the Department of Student Life, Services for Students with Disabilities in Cain Hall, Rm. B118, or call 845-1637.  

"An Aggie does not lie, cheat or steal, or tolerate those who do."