

# CHEM 647-600: Spectroscopic Methods in Organic Chemistry

## Spring 2014 SYLLABUS

T/Th 8:00-9:15 am, CHAN 2122

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<b>PROFESSOR:</b>	<b>Dr. Janet Bluemel</b> —Reed McDonald building (RMD), room 323 (via 321) PHONE: 979-845-7749   E-MAIL: <a href="mailto:bluemel@tamu.edu">bluemel@tamu.edu</a> Homepage Bluemel: <a href="http://www.chem.tamu.edu/rgroup/bluemel/">http://www.chem.tamu.edu/rgroup/bluemel/</a>
<b>OFFICE HOURS:</b>	<b>T/Th 9:30-11:00 am</b> , or by appointment
<b>TEACHING ASSISTANT:</b>	<b>Kyle J. Cluff</b> —RMD, room 428 or 402 (both via room 428) PHONE: 979-862-7826   E-MAIL: <a href="mailto:kyle.cluff@chem.tamu.edu">kyle.cluff@chem.tamu.edu</a>
<b>ASSISTANT:</b>	<b>Jennifer Belcik</b> —RMD, room 321, only afternoons, 1-5 pm PHONE: 979-845-3786   E-MAIL: <a href="mailto:jbelcik@tamu.edu">jbelcik@tamu.edu</a>

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### TEXTBOOKS:

#### Indispensible for Chemistry Students:

- "Organic Structural Spectroscopy", Joseph B. Lambert, Herbert F. Shurvell, David A. Lightner, R. Graham Cooks, Prentice Hall, Upper Saddle River, New Jersey 07458, 2<sup>nd</sup> Edition 2011, ISBN: 0-13-258690-8
- "Organic Structures from Spectra", L. D. Field, S. Sternhell, J. R. Kalman, Wiley & Sons, Ltd, 5<sup>th</sup> Edition 2002, ISBN: 0-470-84362-4
- "Organic Structure Analysis", Phillip Crews, Jaime Rodriguez, Marcel Jaspars, Oxford University Press, 1<sup>st</sup> Edition 1998, ISBN: 0-19-510102-2

#### Students from other departments might also want to look into:

- "NMR for Physical and Biological Scientists", Thomas C. Pochapsky, Susan S. Pochapsky, Taylor & Francis, New York, London, 1<sup>st</sup> Edition 2007, ISBN: 0-8153-4103-2
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### COURSE GRADING:

<b>Midterm Exam I</b> (Thursday, March 6, 2014, 8:00-9:15 am, CHAN 2122)	20%
<b>Midterm Exam II</b> (Tuesday, April 8, 2014, 8:00-9:15 am, CHAN 2122)	30%
<b>Final Exam</b> (Monday, May 5, 2014, 1:00-3:00 pm, CHAN 2122)	50%

### 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 regarding 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.

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### 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. Analytical Methods in Organometallic Chemistry

- (1) Multinuclear and organometallic NMR spectroscopy
  - common spin-1/2 nuclei, e.g.  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{29}\text{Si}$ ,  $^{119}\text{Sn}$
  - quadrupolar nuclei, e.g.  $^2\text{H}$ ,  $^6\text{Li}$ ,  $^{11}\text{B}$ ,  $^{14}\text{N}$
- (2) NMR of diamagnetic organometallic compounds
  - peculiarities of  $^1\text{H}/^{13}\text{C}$  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

### 2. Most Recent Applications of NMR, IR, and UV/VIS

- as found in new publications during the course
  - presented by visitors in lectures
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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 two written midterm exams, and one written final exam, which count 20, 30, and 50% of the overall grade. Additionally, there are many homework sets that will be 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 of molecular compounds.

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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."*