Southeast Missouri State University
Course Syllabus

Department of Chemistry

Course No. CH447/647
Revised Spring 2005

Title of the Course: **Advanced One and Two-Dimensional Nuclear Magnetic Resonance (NMR) Techniques**

- **Catalog Description and Credit Hours:** Advanced Nuclear Magnetic Resonance (NMR) techniques applied to structure determination. This course will provide theoretical and hands-on-training of various 1D and 2D NMR techniques. Two hours of lecture and two hours of laboratory per week (3 credit hours).

- **Prerequisites:** Organic Chemistry II Lab (CH344) or consent of instructor.

- **Purpose or Objectives of the Course:** Fourier-transform high field NMR spectroscopy techniques have evolved to become the principal instrumental technique to elucidate structure of organic compounds. This course will discuss the theoretical basis for and will provide hands-on-training for a number of NMR techniques.

- **Expectations of Students:** Students are expected to learn various NMR techniques demonstrated in the lab and be able to apply them to deduce structure of organic compounds assigned to them as unknown sample.

	Course Outline	**No. of Class Hours**
Week 1-3	**Introduction to High Field NMR**	6
	Nuclear spin and resonance, rotating frame of reference, pulses, spins, spin relaxations, mechanism for spin relaxation.	
Week 4-6	**Practical aspects of high resolution NMR**	6
	An overview of NMR spectrometer, data acquisition, data processing, preparing the sample, NMR standards, preparing the spectrometer, locking, shimming.	
	Exam 1	
Week 7-9	**One Dimensional Nuclear Magnetic Resonance Spectroscopy**	6
	One Dimensional Technique The single pulse experiment Optimizing sensitivity Quantitative measurement and integration	

Spin decoupling methods: homonuclear and hetero-nuclear decoupling

Week 10-11 **Sensitivity Enhancement and Spectral Editing** 4

Polarization transfer
Distortionless Enhancement of Polarization Transfer (DEPT)
Insensitive Nuclei Enhanced by Polarization Transfer (INEPT)

Exam 2

Week 12-15 **Two Dimensional Nuclear Magnetic Resonance Spectroscopy** 8

Introduction to 2D NMR

Quadrature detection
2D data acquisition
2D data processing

Correlation through Chemical Bonds:

Homonuclear Correlation Spectroscopy (COSY)
Double Quantum Filtered Correlation Spectroscopy (DQFCOSY)
Total Correlation Spectroscopy (TOCSY)
Incredible Natural Abundance Double Quantum Transfer Experiment (INADEQUATE)
Heteronuclear Correlation Spectroscopy (HETCOR)
Heteronuclear Multiple Bond Correlation (HMBC)
Heteronuclear Multiple Quantum Correlation (HMQC)
J-Resolved Spectroscopy

Correlation Through Space:

Nuclear Overhauser Effect (NOE)
2D Nuclear Overhauser Effect (NOESY)

Exam 3

- **Laboratory outline** **No. of Class Hours**

Week 1 Introduction, Login, creation of a new data file and file manipulation on NMR dedicated computer. 2

Week 2 Probe Tuning and Matching, Locking, Shimming and Cryogen Filling. 2

Week 3	Standard proton NMR: Data Acquisition, Processing and Plotting.	2
Week 4	Pulse Calibration.	2
Week 5	Relaxation (T_1) Measurement.	2
Week 6	Standard Carbon NMR Data Acquisition, Processing and Plotting.	2
Week 7-8	Homonuclear Decoupling Experiment: Decoupler Power Calibration, Data Acquisition, Data Processing, and Plotting.	4
Week 9-11	Carbon NMR Experiment without ^{1}H Decoupling.	6
Week 12-13	2D Homo-Correlation Spectroscopy (COSY): data acquisition, data processing, and plotting 2D COSY spectrum.	4
Week 14-15	2D Hetero-Correlation Spectroscopy (HETCOR): data acquisition, data processing, and plotting 2D HETCOR. Checkout.	4

Students in CH647 will receive two samples of unknown organic compound for structure determination. They will utilize one-dimensional NMR techniques to establish structure of one of the samples and one- and two-dimensional NMR techniques for the second unknown compound whose structure will be more complex than the first sample. Determination of the structure of the second unknown compound will give graduate students training in this field similar to that required to characterize pharmaceutical compounds developed during new drug discovery. In addition, students in CH647 will submit a research paper on an advanced NMR technique utilized frequently by chemists employed in pharmaceutical and chemical industries.

- **Textbook and supplies:**

  (a) High Resolution NMR Techniques in Organic Chemistry; Timothy D. W. Claridge, Pergamon, 1999.
  (b) Handouts.

- **Basis of Student Evaluation**

  The weight of evaluation criteria may vary at the discretion of the instructor and will be indicated at the beginning of each course.

(CH647)

Homework	10%
Exams	40%
Laboratory work	40%
Research Paper	10%

Tentative Grading scale:

90 – 100%	A
80 – 89%	B
70 – 79%	C
< 69%	F

- Programs Served by this Course: All Chemistry MNS degree program**.**

Violations of academic honesty represent a serious breach of discipline. Engaging or knowingly assisting in academic dishonesty, including plagiarism, cheating, and those acts which would deceive, cheat, or defraud so as to promote or enhance one's scholastic record may be considered grounds for disciplinary action. Please refer to http://www6.semo.edu/judaffairs/code.html for the complete policy on Academic Honesty at Southeast Missouri State University.