

**SYLLABUS for CH 841 and CH 841L**  
**Fall 2009**

**Chemical Applications of NMR Spectroscopy**

**Catalog Description:** Basic concepts of NMR spectroscopy with application to organic, inorganic, physical, and analytical chemistry are discussed. Design of spectroscopic experiments and interpretation of the spectra will be reviewed. Modern experimental techniques include multipulse, multinuclear and multi-dimensional methods, as well as pulsed field gradients.

**Credits:** 3(2,2)

**Prerequisites:** Undergraduate courses covering modern spectroscopic techniques including NMR or consent of the instructor. Basic knowledge in organic chemistry is assumed.

**Textbook :** None required. J.K.M. Sanders, B.K. Hunter "Modern NMR spectroscopy. A guide for chemists" (optional) or Timothy Claridge "High-Resolution NMR Techniques in Organic Chemistry" (optional).

**Course Coordinator:** Dr. Alex Kitaygorodskiy (Alex Kitt),  
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**Where:** Hunter 470 (lectures), 225 and 247A (labs)

**When:** **Lectures** M, W, F (11:15-12:05).  
**Labs** To be arranged in accordance with the instruments' schedule.

**Attendance Policy:** Regular and punctual attendance at all class and laboratory sessions is a student obligation, and each student is responsible for all the work, including tests and written work, in all class and laboratory sessions.

**Objectives:** The course is designed to provide an overview of applications of NMR spectroscopy in chemistry with

emphasis on modern experimental techniques and data interpretation.

**Academic Integrity** As members of the Clemson University community, we have inherited Thomas Green Clemson's vision of this institution as a „high seminary of learning”. Fundamental to this vision is a mutual commitment to truthfulness, honor, and responsibility, without which we cannot earn the trust and respect of others. Furthermore, we recognize that academic dishonesty detracts from the value of a Clemson degree. Therefore, we shall not tolerate lying, cheating, or stealing in any form.

**Disability access statement from the Office of Student Disability Services:**

"It is University policy to provide, on a flexible and individualized basis, reasonable accommodations to students who have disabilities. Students are encouraged to contact Student Disability Services to discuss their individual needs for accommodation."

## Topical Outline

### Experimental Aspects of Modern NMR Spectroscopy

- a. The one pulse experiment: free induction decay (FID); quadrature detection; pulse width; hard and selective pulses; field lock; experiment optimization; etc.
- b. Data processing: Fourier transformation; apodization functions; phasing; integration; linear prediction.
- c. NMR relaxation. Connections through space. NOE effect in NMR. Spin-coupling. Polarization transfer between coupled nuclei.
- d. Multi-pulse experiments: inversion recovery (T<sub>1</sub> measurements); spin echoes and transverse relaxation. INEPT; DEPT.
- e. The second dimension (2D NMR): Quantum-mechanical approach; coherence transfer; phase cycling and coherence selection; COSY and its versions, TOCSY, HETCOR, NOESY, HMQC, HSQC, etc.
- f. Gradient selected spectroscopy. Solvent suppression. Coherence selection. Diffusion studies.

g. Special considerations for biological applications of NMR: TROSY; 3D-spectroscopy

### **NMR Applications in Organic Chemistry**

- a. The chemical shift
- b. Spin-spin coupling
- c. Time dependent phenomena
- d. Relaxation
- e. Carbon NMR
- f. Paramagnetic molecules
- g. Polymers

### **Introduction into Solid State NMR.**

### **Multinuclear NMR**

**Evaluations:** Midterm test (35%), Final exam (35%), Home assignments + quizzes (20%), Problem set (10%).