Practical NMR Spectroscopy

Course Description: Magnetic Resonance Spectroscopy is a powerful technique that has evolved with applications in virtually every scientific discipline. This course focuses on the application of NMR Spectroscopy to the structure determination and dynamics of primarily synthetic organic and organometallic products. Although automation of NMR data collection is becoming mainstream, the practical aspects of acquiring optimized, high-quality data are still beneficial for analysis of these spectra. Various aspects of optimization will be covered such as pulse calibrations, probe tuning, measuring relaxation parameters, sample preparation, and shimming. The applications of these techniques to a variety of routine NMR experiments will be demonstrated, as well as advanced sequences in an attempt to make seemingly complex experiments more accessible to the synthetic chemist to simplify structure determination. The course will be a combination of short lectures with demonstrations utilizing the department's NMR facility instrumentation. Previous use of the facility instruments is recommended.

Meeting times: The class will meet twice a week for one hour and 20 minues.

I. Week One

NMR Theory
Magnetic moment, NMR transition and spin states, vectors and RF pulses
Relaxation parameters, T_1 and T_2

The NMR
Probes and tuning, magnet and cryogens, RF routing, and the workstations
Safety and NMR

Experimental parameters
Sample handling, locking and shimming
Optimizing signal to noise, gain, pulse widths, line-widths
Acquisition of basic proton NMR spectrum

Demo
Sample handling, locking and shimming
Optimizing signal:noise, pulse calibrations
Acquiring your best NMR spectrum

II. Week Two

More 1D methods
Edited 1D spectra
Dipolar coupling, ie. The NOE
Quantitative NMR is possible

Multinuclear NMR
Relative sensitivity, quadruple nuclei
Acquisition of multinuclear NMR spectrum

Data Processing
Multiplet analysis
Phasing, baseline corrections, line broadening
Tips and Tricks

Demo
Quantitative NMR
Homonuclear decoupling
Acquisition of ^{31}P and ^{19}F NMR

III. Week Three

Multidimensional NMR
2D NMR pulse sequences
Optimization of 2D NMR acquisition

Demo
^{1}H – ^{1}H Correlation spectroscopy
^{1}H – ^{13}C Heteronuclear spectroscopy

IV. Week Four

Miscellaneous
Selective Pulses
Diffusion
Solid-state NMR

Demo
$T_1(H)$ measurement and processing
Selective NOE setup and measurement
Student choice

Prerequisites: Organic Spectroscopy (Chem 5420) or by consent of the Instructor.

Grading: Grading is based on two exams (70%) and participation (30%).

Recommended reading list:

Keeler, J.; Understanding NMR Spectrscopy, Wiley, **2010**.

Levitt, M.; Spin Dynamics; Basics of Nuclear Magnetic Resonance, Wiley, **2008**.

Silverstein, R. M.; Webster, F.X.; Kiemle, D.; Spectrometric Identification of Organic Compounds, Wiley, **2005**.

Berger, S.; Braun, S.; 200 and More NMR Experiments; A Practical Course, Wiley-VCH, **2004**.

Mason, J. E. Multinuclear NMR, Springer, **1987**.

It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term “academic misconduct” includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct http://studentlife.osu.edu/csc/.

Students with disabilities that have been certified by the Office for Disability Services will be appropriately accommodated and should inform the instructor as soon as possible of their needs. The Office for Disability Services is located in 150 Pomerene Hall, 1760 Neil Avenue; telephone 292-3307, TDD 292-0901; http://www.ods.ohio-state.edu/.