

CHEM 618: NMR SPECTROSCOPY

SPRING 2009 SYLLABUS

Professor Janet Bluemel

Tuesday and Thursday: 2:20 pm-3:35 pm, CHAN 2101

This course will cover modern one and two-dimensional NMR techniques for liquids, suspensions, and solids. The emphasis will be on multinuclear NMR applications on a wide range of compounds and materials that are interesting in inorganic, organometallic, and biological chemistry.

Students will be provided with course material (lecture and exercise material), and printouts of the power point files. Any textbook covering the basics of NMR spectroscopy, such as the book by H. Friebolin, *Basic One- and Two-dimensional NMR Spectroscopy*, will be a useful, additional reference for this course. There will be one written midterm, and one written final exam—both count 1/3 of the overall grade. There are also eight homework sets that count 1/3 for the grade. Students are also welcome to bring NMR problems from their own Ph.D. work to be discussed.

I. NMR Spectroscopy of Liquids

(1) Brief Repetition: The Basics of One and Two-Dimensional NMR Spectroscopy

- the NMR experiment and the main parts and functions of the NMR spectrometer
- the chemical shift and proper referencing with internal and external standards
- the J-coupling and standard correlation spectroscopy
- processing NMR spectra
- more special pulse sequences and tricks

(2) Multinuclear NMR Spectroscopy

- the more common spin-1/2 nuclei, e.g., ^{19}F , ^{31}P , ^{29}Si , ^{119}Sn
- quadrupolar nuclei, e.g., ^2H , ^6Li , ^{11}B , ^{14}N , and their characteristics and applications

(3) NMR of Diamagnetic Organometallic Compounds

- peculiarities of $^1\text{H}/^{13}\text{C}$ chemical shifts
- different J-coupling scenarios and virtual couplings
- dynamic effects and ligand exchange

(4) Paramagnetic NMR Spectroscopy

- the basics of paramagnetic compounds and their NMR
- tricks and examples of organometallic compounds and materials

II. NMR Spectroscopy of Solids

(1) Interactions in the Solid State

- the 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)
- equipment for special modern techniques, e.g., surface coils

III. Most Recent Applications of Liquids and Solids NMR

(1) Homogeneous and Heterogeneous Catalysis

- HRMAS of suspensions (polymers, dendrimers, substances bound on surfaces)
- dipolar dephasing, diffusion spectroscopy

(2) Inorganic and Organometallic chemistry

- solid-state NMR of materials (metal organic frameworks (MOFs), chromatography phases)
- exchange processes and in situ reactions

(3) Applications of Solid-State NMR Spectroscopy in Biochemistry (membranes, proteins)