Chemistry 626: NMR Spectroscopy in Chemistry and Biochemistry
Instructor: Anthony S. Serianni

Abbreviated Syllabus
Spring 2006

Lecture Component

The NMR Phenomenon
Historical; difference between CW and FT modes of data collection
Comparison of NMR to other forms of spectroscopy: sensitivity
Review of fundamental NMR parameters
Static: chemical shift; spin-spin couplings (^1J, ^2J, ^3J, ^4J, ^5J); Karplus relationships;
homonuclear and heteronuclear couplings; non-first-order effects
Dynamic: spin-lattice and spin-spin relaxation; nuclear Overhauser enhancement;
relaxation mechanisms

Discussion of laboratory and rotating frames; vector models of pulses
Effect of applying an rf pulse using vector model
Introduction to the product-operator formalism
Vector models to describe chemical shift and spin-coupling behavior
Pulse phasing ($\pi/2_x$, $\pi/2_y$, $\pi/2_{-x}$, $\pi/2_{-y}$)
Multipulse methods in one dimension: inversion-recovery method; spin echoes; CPMG pulse sequence
Refocusing pulses (chemical shifts; spin-couplings)
Nuclear Overhauser effect: role of zero, single and double quantum transitions; steady-state nOe; three-spin effects; transient nOe; homonuclear and heteronuclear nOes; gated decoupling
Interproton distance measurements by DESERT
Polarization transfer: selective population transfer (SPT); INEPT; refocused INEPT; DEPT; reverse DEPT

Hard and soft pulses
Calibrating pulse widths (observe coil)
Calibrating pulse widths (decoupling coil)
Determining decoupler field strength (homonuclear; heteronuclear)
Dealing with imperfect pulses: composite pulses; WALTZ decoupling; GARP; WURST
Relationship between pulse width and repetition rate
Problems of quantitation by NMR
Tailored excitation for solvent suppression: Redfield 214 pulse; JR method; pulse shaping

Selective excitation: soft square pulses; pulse shaping; DANTE
Applications of pulsed field gradients (PFG); gradient-enhanced spectroscopy
2D NMR Spectroscopy
    COSY; COSY45; DQF-COSY; TQF-COSY; E-COSY; INADEQUATE (1D, 2D);
    NOESY; ROESY; 2D exchange spectroscopy (saturation and inversion transfer);
    J-spectroscopy (homonuclear, heteronuclear); HETCOR; HMQC; HMBC; HOHAHA (TOCSY)
BIRD and TANGO pulses
3D NMR spectroscopy
    Homo- and heteronuclear versions (HMQC-TOCSY, HCCH-TOCSY)
4D NMR Spectroscopy

Physical basis of nuclear relaxation
Effect of molecular motion on T_1, T_2, nOe
Dipole-dipole mechanism of relaxation
Quadrupolar relaxation
Relaxation via spin-rotation and chemical shift anisotropy (CSA)
Segmental motion
Quantitative evaluation of chemical exchange processes by NMR (Gutowsky-Holm method; magnetization transfer; 2D exchange spectroscopy)

Effect of stable isotopic enrichment on NMR spectra; spectral editing via stable isotopes
Enrichment methods: ^{13}C, ^{15}N, ^{2}H
Oligopeptide/protein structure determination by NMR
Oligonucleotide structure determination by NMR; problem of conformational averaging
Carbohydrate structure determination by NMR

Solid-state NMR: cross-polarization; magic angle spinning
REDOR spectroscopy

Miscellaneous applications
    In vivo spectroscopy; MRI, MRS
    Measuring intracellular pH by ^{31}P and ^{19}F NMR
    Surface coils; magnetic resonance imaging; NMR microscopy
    Metabolic monitoring by NMR with stable isotopes
    Studies of enzyme mechanisms by NMR