SYLLABUS – CHM6580, Spring 2018

Introduction to Spin Dynamics and Nuclear Magnetic Resonance

Instructor: Russ Bowers, Department of Chemistry
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Office Hours: MWF, 1:30-3:00 pm
Class meeting times: Tuesday period 2; Thursday periods 2-3
Place: Flint 0109

OBJECTIVES

The theory and practice of time-domain nuclear magnetic resonance spectroscopy is introduced, beginning with the quantum mechanics of spin, spin interactions, coherence, and relaxation. Experimental aspects include time-domain signal acquisition, signal conditioning/processing, properties of Fourier transforms, resonant radio-wave circuits, NMR spectrometer architecture, and pulse sequences for NMR in one and two-dimensions. Levitt's SPINDYNAMICA package (running in Wolfram's Mathematica) is used extensively throughout the course.

PREREQUISITES

No prior knowledge about NMR is assumed. All concepts are developed from first principles. A prior course on quantum mechanics is recommended.

PLACE IN CURRICULUM

This course satisfies the spectroscopy core requirement to qualify for the PhD in the Physical Chemistry Division.

REQUIRED TEXTS

- Malcolm H. Levitt, Spin Dynamics: Basics of Nuclear Magnetic Resonance (Paperback), Wiley; 2nd edition, ISBN-13: 978-0470511176
- James Keeler, Understanding NMR Spectroscopy (Paperback), Wiley, 2nd edition, ISBN-13: 978-0470746080

REQUIRED SOFTWARE

- Wolfram's Mathematica (version 8 or higher)
- Malcolm Levitt's Spindynamica package (http://www.spindynamica.soton.ac.uk/)

OPTIONAL SOFTWARE

- MestReNova (UF Chemistry site licensed)
- Bruker Topspin (Student edition available, https://store.bruker-biospin.com/shop/US/product/H9966S3/)

SUPPLEMENTAL TEXTS (USED TO PREPARE LECTURES)

- Richard R. Ernst, Geoffrey Bodenhausen, Alexander Wokaun, Principles of Nuclear Magnetic Resonance in One and Two Dimensions (Paperback), Oxford University Press, ISBN-13: 978-0198556473
- B.C. Gerstein and C.R. Dybowski, Transient Techniques in NMR of Solids: An Introduction to Theory and Practice, Academic Press, Inc. (1985) ISBN: 0-12-281180-1.
- M. Duer, Introduction to Solid-State NMR Spectroscopy, Wiley-Blackwell, 1st Edition (2005) 978-1405109147.

GRADING: in-class exam (30%), take-home exam (30%), labs (20%), homework (20%). Letter grades will be assigned based on the following tentative scheme:

>80 %	A
>75 %	A-
>70 %	B+
>60 %	B
>50 %	C

ATTENDANCE: 100% attendance and class participation are expected.

MAKE-UP EXAMS: Must be arranged in advance of the scheduled date. Make-up exams allowed only in emergency situations.

UF GENERAL INFORMATION A GRADES:
https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

TENTATIVE SCHEDULE

SPIN QUANTUM MECHANICS	
1	Two level systems, resonant absorption, spin angular momentum, magnetic dipole moments, spin polarization axis, spin magnetization.
2	Spin precession, torque equation, B_1 field, Bloch equations.
3	Rotating frame Bloch equations, vector picture, steady-state magnetization, continuous-wave NMR, absorption, dispersion functions.
4	Spin quantum numbers, spin states, Dirac notation, Zeeman interaction.
5	SPINDYNAMICA tutorial I.
6	Eigenvalue equations, Hermitian operators, unitary operators, powers of operators, exponentials of operators, commutator of spin operators, raising and lowering operators, trace properties, rotation operators
7	Matrix representation of operators, RF pulses, nutation, RF offset effects
8	Density operator, density matrix, populations, coherences, orders of coherence, coherence transfer, thermal equilibrium density operator.
9	Liouville-von Neumann equation, rotating frame density operator, coherence excitation, population inversion, free induction decay.
10	SPINDYNAMICA tutorial II. Spectral simulations.
SIGNAL ACQUISITION AND PROCESSING	
11	Digitization, Receiver reference, phase shift, linear phase shift, Nyquist theorem
12	NMR hardware, spectrometer block diagram, probe circuits, duplexer, receiver, transmitter
13	Signal processing: left shift, baseline correction, zero-fill, apodization
14	The Fourier Transform, convolution theorem
15	Artefacts, quad-ghosts, phase correction, peak integration, processing real NMR data
COUPLED SPIN SYSTEMS	
16	Spin coupling, quantum states of coupled spins, diagonalization, singlet/triplet basis, Zeeman basis, signals calculation for arbitrary coupling, tensor product, pure states, entangled states
17	multi-spin density operator, master equation
18	product operator formalism 1: AX spin system
19	product operator formalism 2: AX_2, AX_3 spin systems, propagators, propagator manipulations, composite pulses, signal calculations.

MULTIDIMENSIONAL SPECTROSCOPY	
20	Spin echo and J-spectroscopy
21	Chemical Exchange Spectroscopy (2D-EXSY)
22	INEPT (non-refocused), INEPT (refocused), exchange spectroscopy
23	Phase cycling, coherence transfer pathway selection, homospoil
24	COSY, DQF COSY, TOCSY
25	HMQC, HSQC, DOSY
RELAXATION	
26	random field relaxation, fluctuations, spectral density, transition probability
27	relaxation mechanisms, chemical shift relaxation, homonuclear dipole-dipole relaxation, heteronuclear dipole-dipole, quadrupolar relaxation
28	relaxation measurements, inversion recovery, CPMG-T2
29	NOESY
SOLIDS, RELAXATION THEORY	
30	Spin interactions in solids: chemical shift, dipole-dipole, electric quadrupole, “secular” vs. “non-secular” interactions
31	Chemical shift tensors, powder patterns in static spectra, principle value extraction.
32	Solid-echo, Magic Angle Spinning, Cross-Polarization.

LAB #1	RF lab: oscilloscope, network analyzer, splitters, mixers, hybrids, directional couplers, attenuators, phase shifts, duplexer, impedance matching and probe circuit tuning.
LAB #2	Fun with spin echoes: Hahn echo, solid-echo, stimulated echo.
LAB #3	Solid-state NMR, 13C/1H Cross-Polarization Magic Angle Spinning.