# SYLLABUS – CHM6580, FALL 2015

*Introduction to Spin Dynamics and Nuclear Magnetic Resonance*

**Instructor:** Prof. Russ Bowers, Department of Chemistry, University of Florida
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**Office Hours:** TBA
**Class meeting times:** T period 2**,** R periods 2-3
**Place:** NPB 1200

## OBJECTIVES

Students are introduced to the theory and practice of modern nuclear magnetic resonance spectroscopy in liquids and solids. Students will gain a fundamental understanding of spin interactions, spin coherence, and spectroscopy. Experimental aspects are also covered, including signal acquisition and processing, properties of Fourier transforms, probe circuits, and spectrometer design. Levitt's SPINDYNAMICA package (running in Wolfram's Mathematica) is used extensively throughout the course. There will be two hands-on experimental labs giving students an opportunity to learn the basics of RF electronics.

## PREREQUISITES

No prior knowledge of NMR is assumed. Knowledge of quantum mechanics and Mathematica programming is helpful but not required.

## 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.
- Abragam, Principles of Nuclear Magnetism, Eds. W.C. Marshall and D.H. Wilkinson, Oxford University Press, New York,(1985) ISBN 0-19-852014 X Pbk.

**GRADING:** in-class exam (30 %), take-home exam (30 %), labs (20 %), homework (20 %).
**ATTENDANCE:** 100% attendance is expected.
**MAKE-UP EXAMS:** Must be arranged in advance of the scheduled date. No make-up exams are allowed otherwise.
**UF GENERAL INFORMATION A GRADES:** https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

| **LECTURE** | |
|---|---|
| 1 | two level systems, resonant absorption, spin angular momentum, dipole moments, spin polarization axis, spin magnetization |
| 2 | spin precession, torque equation, Bloch equations, relaxation, rotating frame |
| 3 | rotating frame Bloch equations, $B_1$ field, vector picture, steady-state magnetization, continuous-wave NMR, absorption, dispersion functions. |
| 4 | spin quantum numbers, spin states, Dirac notation, Zeeman interaction, relationship of quantum and classical magnetic moments. |
| 5 | Introduction to SPINDYNAMICA |
| 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 | ensembles of spins, density operator, populations, coherences, orders of coherence, coherence transfer, thermal equilibrium density operator, Liouville-von Neumann equation |
| 9 | rotating frame density operator, coherence excitation, population inversion, free induction decay, signal calculation |
| 10 | phase shifts, receiver reference, linear phase shift, Nyquist sampling theorem, Fourier transform |
| 11 | NMR hardware, spectrometer block diagram, probe circuits, duplexer, receiver, transmitter, digitization |
| 12 | Signal processing: left shift, baseline correction, zero-fill, apodization, quad-ghosts, phase correction, peak integration, processing real NMR data. |
| LAB #1 | RF lab: oscilloscope, network analyzer, splitters, mixers, hybrids, directional couplers, attenuators, phase shifts, duplexer, impedance matching and probe circuit tuning. |
| 15 | Coupled spin systems in liquids, quantum states of coupled spins, diagonalization, singlet/triplet basis, Zeeman basis, signals calculation for arbitrary coupling, tensor product, pure states, entangled states. |
| 16 | multi-spin density operator, master equation |
| 17 | product operator formalism 1. |
| 18 | product operator formalism 2: $AX_2$, $AX_3$ spin systems, propagators, propagator manipulations, composite pulses, signal calculations. |
| 19 | pulse Sequences 1: spin echo, J-spectroscopy |
| 20 | pulse Sequences 2: INEPT (non-refocused), INEPT (refocused), exchange spectroscopy |
| 21 | phase cycling, coherence transfer pathway selection, homospoil |
| 22 | pure absorption 2D spectra, COSY, TOCSY, |
| 23 | spin interactions in solids: chemical shift, dipole-dipole, electric quadrupole, “secular” vs. “non-secular” interactions |
| 24 | solid-state NMR: chemical shift powder patterns, Pake patterns, quadrupolar powder patterns, principle value extraction |
| LAB #2 | Fun with spin echoes: Hahn echo, solid-echo, stimulated echo. |
| 27 | random field relaxation, fluctuations, spectral density, transition probability |
| 28 | relaxation mechanisms, chemical shift relaxation, homonuclear dipole-dipole relaxation, heteronuclear dipole-dipole, quadrupolar relaxation |
| 29 | relaxation measurements, inversion recovery, CPMG-T2 |
| 30 | NOESY spectroscopy, distance measurements |
| 31 | chemical exchange effects, 1D exchange spectroscopy, 2D exchange spectroscopy |
| 32 | Solid-state NMR (magic angle spinning), cross-polarization, dipolar decoupling |
| 33 | hyperpolarization methods 1:DNP, optical pumping |
| 34 | hyperpolarization methods 2: parahydrogen induced polarization |