Chemistry 59-542/445: NMR Spectroscopy Fall 2016 Semester v. 1.0

General Information

Professor:	Rob Schurko
Office:	389 Essex Hall
Email:	rschurko@uwindsor.ca
Website:	http://www.uwindsor.ca/schurko
Lecture Times:	Two 75 min. lectures per week, to be scheduled with students
Tutorials:	Prior to examinations
Assignments:	Seven assigned problem sets, not handed in for marks. Six short assignments to keep students up to date with course materials.

I. Instructional Materials

The course is largely based upon the notes which are handed out in each class. Students receive approximately 25 sets of notes and 7 sets of tutorial problems.

Textbooks (optional):

There is not a mandatory textbook for the course; suggested readings come from:

1. Keeler, J. *Understanding NMR Spectroscopy*. John Wiley & Sons, Chichester, U.K, 2005 ISBN 13978-0-470-01786-9 (soft cover).
2. Hore, P.J.; Jones, J.A. and Wimperis, S. *NMR: The toolkit.* Oxford University Press, Oxford, U.K., 2000. An Oxford Chemistry Primer. ISBN 0 19 8504152 (soft cover)
3. Levitt, M.H. *Spin Dynamics: Basics of Nuclear Magnetic Resonance.* John Wiley & Sons, New York, 2001. ISBN 0471489220 (soft cover)
4. Claridge, T.D.W. *High-Resolution NMR Techniques in Organic Chemistry*. Elsevier Science, The Netherlands, 1999. ISBN 0080427987 (soft cover).

II. Course Objectives

1. To provide the student with an understanding of the physical basis of NMR, all the way from nuclear spin to modern two-dimensional NMR techniques.
2. To train the student in the practical aspects of NMR spectroscopy, including spectral processing and NMR hardware.
3. To encourage the student to utilize a wide variety of NMR experiments and techniques to aid in their ongoing research.

III. Tutorials and Laboratories

Tutorial sessions are offered prior to all quizzes and/or examinations. There is currently no laboratory component for this course, though several laboratory demonstrations are given.

Mark breakdown and guidelines

Mark Breakdown:	**59-542**	**59-445**	
Mid-term 1	15%	20%	TBA
Mid-term 2	15%	20%	TBA
Assignments	10%	10%	
Presentation	20%	--	TBA
Final Exam	40%	50%	TBA

Note: Lecture slots and exam times will be scheduled in the first week of classes with the consent of all students in 59-445 and 59-542. I will try my best to work around all scheduling issues for all students.

A. Attendance is VERY IMPORTANT to be successful in this course - students who do not attend lectures generally score very low on quizzes and exams. **You must keep up with the material as the semester progresses.**

B. To arrange consultation time with Dr. Schurko, please **make an appointment by email**. Office hours are quite flexible and will be adjusted around your schedule of classes and t.a. responsibilities.

C. Updated versions of lecture notes will be handed out at the start of class, and adequate lecture notes should be taken as a compliment. Students are encouraged to consult with the instructor about any material that is unclear.

D. Problem sets are handed out as the course progresses, and are directly related to material from the notes. Answer keys are available for these problem sets.

E. This year, six short assignments will be handed out to keep the students up to date with course materials.

F. Exams missed due without an official excused absence will result in a grade of zero. Only students with an official excused absence will be given the opportunity to make-up an exam, which may be written or oral. If for health or personal reasons an exam must be missed, you must notify Dr. Schurko by phone or email within 12 hours before or after the exam.

G. All students are required to take the final examination in order to receive a passing grade in the course. No notebooks, texts or cheat sheets are allowed in any of the examinations. Students caught cheating will receive an automatic grade of zero and be subject to academic discipline.

Outline of Course Material

Section 1: Introduction to NMR
Lecture 1: NMR in Context: Spectroscopy; History of NMR; Nuclear Spin
Lecture 2: Vector Model, Semi-Classical Model, Rotating Frame
Lecture 3: Quantum Mechanics of NMR
Lecture 4: Spin Operators
Lecture 5: Density Matrix Theory: Populations and Coherences

Section 2: Fourier Transform NMR & The NMR Spectrometer
Lecture 6: The Basic FT NMR Experiment
Lecture 7: The Fourier Transform in NMR
Lecture 8: Spectral Processing and Data Manipulation
Lecture 9: The NMR Spectrometer; Practical Considerations
Lecture 10: Phase Cycling and Pulse Sequences

Midterm 1

Section 3: NMR Interactions, Relaxation and Chemical Exchange
Lecture 11: NMR Interactions: Introduction, Quadrupolar Interaction
Lecture 12: Chemical Shielding
Lecture 13: Direct Dipole-Dipole Interaction
Lecture 14: Indirect Spin-Spin Interaction (J-Coupling)
Lecture 15: Relaxation in NMR
Lecture 16: Relaxation Mechanisms and Dynamic Motions
Lecture 17: Chemical Exchange Phenomena

Section 4: Advanced Topics in NMR
Lecture 18: Coherences and the AX Spin System
Lecture 19: Double Resonance Experiments, Part 1
Lecture 20: Double Resonance Experiments, Part 2

Midterm 2

Lecture 21: Introduction to 2D NMR, J-resolved and COSY Experiments
Lecture 22: General Features in 2D NMR
Lecture 23: Survey of 2D NMR Techniques
Lecture 24: Introduction to Solid-State NMR
Lecture 25: Student Presentations: Special Topics in NMR

Examinations

All examination dates will be decided upon in class during the first two weeks.

Last updated: June 1, 2016