Chem 6990B Spring 2024

NMR methods

Instructor: Monika Ivancic
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Office hour:
Mondays from 2pm to 3pm
or by appointment

Lectures: MW 9:40am to 10:30am Patrick Leahy Building 218

Lab sections: TBD during 1st lecture Discovery W103

Suggested Textbooks:

"High-Resolution NMR Techniques in Organic Chemistry" by Timothy D.W. Claridge, Pergamon Press, 2nd edition, 2009

"Modern NMR Techniques for Chemistry Research" by Andrew E. Derome, Pergamon Press, 1987

"Modern NMR Spectroscopy: A Guide for Chemists", Second Edition, by Jeremy K.M. Sanders and Brian K. Hunter, Oxford University Press, 1993

Course description & goals:

This course will introduce students to various concepts in Nuclear Magnetic Resonance (NMR), a spectroscopic method used by chemists, biochemists, biophysicists, material scientists and engineers. Starting with how and why NMR works, we will follow up with what information NMR provides (chemical shift, coupling constants, distance information, dynamics, reaction kinetics, to mention a few) and how implementation of specific experiments leads to answers for our investigations. Approximately 2/3 of the course will focus on the theory behind specific NMR techniques as well as thinking about appropriate experiments to solve our research problems. The other 1/3 of the course will involve lab work and implementation of these experiments on the NMR spectrometer.

Commitment to Diversity, Equity and Inclusion

As part of a university wide effort, I am committed to providing equitable instruction to a diverse set of students. I believe that diversity enhances our teaching and learning abilities, being open to new ideas and new ways of doing things. I believe that the research that is done at a university is more robust when coming from a diverse set of people and I strive to be inclusive of students of all walks of life, no matter your race, religion, ability, gender identity, sexual orientation, national origin, language or culture.

Grading & other info

Homework	50%
Lab attendance	10%
Lecture midterm	10%
Final project (ppm assignments)	10%
Lab final exam	20%

•The UVM NMR lab (Discovery W103) is unlocked Mon to Fri – first one in after 8am until 5pm. After hours your Cat Card should get you in (all chem6990B students should have access). The workstation computer is also located in this lab, is part of the UVM system and you will use your NetID to log onto it.

•Now UVM has a site license to MestreNova, which is the NMR processing software. This site license allows for up to 100 users at UVM to install MNova on their personal laptops/computers. The installation instructions will be provided along with the license file. For the software & license to work, your computer will need to register with the server at least every 90 days. Once you leave UVM, the license will become deactivated.

•Labs will be held on an approximately every other week basis. Homework will be based upon what you learned in lab, so please be on time and *pay attention* during lab. Homework assignments are due as specified on the handouts, generally on Monday evening preceding the next lab. The total score for each homework will be 50 points, with a *weighted penalty (5 points/day) for late homework*.

•Carefully go over each homework assignment *prior to* sitting down at the spectrometer. Understand what the assignment requires you to do and develop a strategy **in advance** to meet the goals of the assignment. Acquire the data ASAP after the lab, so that the procedure is fresh in your head. You will still need to work up the data in MestreNova, so the sooner you have the data, the better. DO NOT wait until just before the homework is due to acquire data for the assignment.

•You will be using a class account on each of the spectrometer computers (login & password will be provided). Make sure you name your data sets starting with your initials OR your last name. Let Monika know if you need a research account on either spectrometer.

•Each chem 6990B student will have access to the spectrometer calendar. The link to this calendar is: http://faces.ccrc.uga.edu/ The group name is 'UVMNMR' and I will use your NetID as a login. Please do not use a secure password for this account, as the folks running the site can see your password (you may use 'chem6990B').

•When signing up for spectrometer time to do homework, keep in mind that researchers still need to get data. If possible, please avoid signing up between 10am and 4pm, M-F. The Bruker calendar has a 30 min time limit that you sign up for the same day.

Spring '24 Chem 6990B: NMR methodology course syllabus instructor: Monika Ivancic

Lab component

January 17	course overview; lab structure & schedule labs NMR spectrometer: magnet, console, computer, probe	
Jan 22 & **24**	NMR active nuclei, principles behind NMR (how and why it works) Principles behind NMR: E-levels, Boltzmann distribution	**lab 1:** ^{1}H 1D on Bruker & using MNova
Jan 29 & 31	Intro to MNova & The vector model of NMR: rotating frame, the pulse & QPD	
February 5 & **7**	The vector model (cont'd): phase cycling, Nyquist & sampling the FID Recording the spectrum: time and frequency domains	**lab 2:** ^{13}C 1D & DEPT on Bruker
Feb 12 & 14	Practical aspects of ^{13}C NMR NOE enhancement vs. Polarization Transfer (DEPT, INEPT)	
February **21**	lab only this week	**lab 3:** ^{19}F & ^{31}P 1D on Bruker
Feb 26 & 28	Chemical shifts and coupling Electron shielding; origin of spin-spin coupling X-nuclei NMR and kinetics by NMR	
March 4 & **6**	**Midterm exam**	**lab 4:** quantitative ^{1}H 1D on Varian

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March 18 & 20	T1 & T2 relaxation; Mechanisms of relaxation Review of calibrating the 90^{o} pulse Intro to 2D NMR; Homo vs. heteronuclear experiments	
March 25 & **27**	COSY vs. TOCSY spectroscopy 1H-1H thru bond experiments	**lab 5:** COSY/TOCSY on Varian
April 1 & 3	1H-1H thru space experiments 2D NOESY vs. ROESY theory and practice	
April 8 & **10**	^{1}H-^{13}C HSQC (1-bond) and HMBC (2,3-bond) Spectroscopy; Experiment setup; data interpretation	**lab 6:** HSQC/HMBC on Varian
April 15 & 17	Dynamic NMR: lineshape analysis vs. Coalescence T; rate constants k_c Intermolecular exchange processes	
April 22 & 24	guest lecturer: biomolecular NMR (or similar) final project demo – molecule assignment using 2D data	
April 29 & May 1	special topics: RDCs, protein NMR, large molecule NMR, DOSY	