Chem. 750 Advanced Topics in Analytical Chemistry: Practical NMR

Spring 2015
Schedule number: 31007

Professor Gregory Holland
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COURSE INFORMATION

Class Days: T
Class Times: 5:30-8:10
Class Location: GMCS-305

Office Hours (and by appointment): R 9:30-11:30
Office Hours Location: GMCS-213C

Course Overview

Chem 750: Advanced Topics in Analytical Chemistry is a graduate level course in Practical NMR. This class is focused on learning the practical aspects of NMR spectroscopy including the basics of NMR, pulse sequence and experimental set-up, data processing and data interpretation. Although some theory will be taught, the primary focus of this class is on 'hands-on' training in NMR spectroscopy. The students will spend a considerable fraction of time processing and analyzing real NMR data with NMR software and some fraction of the class will be spent doing NMR training in the NMR lab. Data collection, data processing and data analysis will be covered. Magnetic Resonance has a plethora of different types of experiments; probe designs, pulse sequences, data collection techniques, and data simulation and modeling methods. The large variety of "methods" in magnetic resonance is often overwhelming for new scientists trying to learn how to setup and perform a specific experiment or process and analyze a specific set of data or spectra. The student's grade will come from two class projects, three tests and one presentation. The primary goal of the class is to train the student to collect, process and interpret NMR spectra and relaxation data and ultimately enable them to utilize NMR in their thesis research and future scientific research careers.

Student Learning Outcomes:

1) Basics of NMR, NMR Lab Safety, hardware overview, sample prep, student copy of NMR processing software.

2) 1D 1H NMR. Setup, ^{2}H lock and shim, processing (FT, EM, phase, zero filling, referencing, peak picking, baseline correction, integration, plotting electronic figure).

3) Pulse sequences, pulse programming and experimental design.

4) Advanced 1D 1H NMR**,** J-splitting, chemical shift, T_1 and T_2 measurement, FID analysis, Nutations, Spectral editing pulse sequences.

5) Heteronuclear NMR, ^{13}C, ^{31}P, ^{19}F, etc.

6) Advanced 1D NMR, solvent suppression, selective excitation, DEPT, APT.

7) Common 2D NMR, COSY, NOESY, HSQC, HMBC, INADEQUATE.

8) Tricks for data collection and processing of 2D NMR, 2D-FT, window functions, apodization, linear prediction.

9) NMR self-diffusion measurements and DOSY methods.

10) Basic solid-state NMR techniques.

Enrollment Information

Prerequisites: There are no specific pre-requisites for this class, but it is a graduate level class, and some knowledge of General, Physical and Analytical chemistry is expected.

Course Materials

Book: *No required book, but there are a number of recommended optional materials listed below.*

Lecture Notes: Lecture notes are available upon request. These notes cover the major topic I will go over, **but may not include problems and examples done on the board, NMR demonstrations conducted with NMR software or 'hands on' training conducted in the NMR lab.** Schemes and schematics described on the board generally will not be posted. You will miss this material if you do not attend class.

Recommended (Optional) Materials: Some Classic NMR Texts.

Principles of Nuclear Magnetism, by A. Abragam, Oxford, 1961; ISBN: 978-0-19-852014-6.

Spin Dynamics, by M.H. Levitt, Wiley, 2001; ISBN: 0-471-48922-0.

200 and More NMR Experiments, by S. Berger and S. Braun, Wiley, 2004; ISBN: 3-527-31067-3.

Experimental Pulse NMR: A Nuts and Bolts Approach, by E. Fukushima and S.B.W. Roeder, Perseus, 1981; ISBN: 0-201-62726-4.

Principles of Nuclear Magnetic Resonance in One and Two Dimensions, by R.R. Ernst, G. Bodenhausen and A. Wokaun, Oxford, 1987; ISBN: 0-19-855647-0.

Protein NMR Spectroscopy, by J. Cavanagh, W.J. Fairbrother, A.G. Palmer, M. Rance, N.J. Skelton, Elsevier, 2007; ISBN13: 978-0-12-164491-8.

Spectrometric Identification of Organic Compounds, by R.M. Silverstein, F.X. Webster and D.J. Kiemle, Wiley, 2005; ISBN: 0-471-39362-2.

Multidimensional Solid-state NMR and Polymers, by K. Schmidt-Rohr and H.W. Spiess, Academic Press, 1994; ISBN: 0-12-626630-1.

Course Structure and Conduct

This course will be taught in a combination of formats including lecture 'chalk talk' format, power point presentation, NMR software in class and some hands on training at the NMR spectrometer. Lecture notes and presentations are available upon request. I expect this class to be somewhat informal where questions can be asked during class, during my office hours or following the lecture. The best advice for this class is to be proactive. Start Class Projects early, come to my office hours if you feel you are falling behind and take advantage of the optional reading.

Course Assessment and Grading

Tests: February 17, March 17 and April 21, in class
Projects: Due March 10 (data will be provided 2 weeks prior)
There will be three short tests during the semester, **each worth 100 points**. There will be 6 questions, **but only 5 that need to be answered to get 100%**. Any points earned above 100% will be carried over to your cumulative total. There will be 2 class projects that will involve processing and analyzing real NMR data and reporting the results as a paper with figures. There will be one 15 minute presentation on a published NMR technique from a Journal article of your choice. The student is encouraged to select a NMR methods paper that is related to his/her thesis research. Your final grade will be based on a maximum of **1000 points**, distributed as follows: 3 tests (100 points each), 2 class projects (200 points each), and 1 presentation (300 pts).

Letter Grade Assignment: Depending on class performance grades may be curved**.** If necessary the class average will be curved upward to a 60% (the lowest B-). The cutoff for an A- will be 780 total points. The cutoff for a B- will be 600 points. The cut off for a C- will be 450 points.

Students with Disabilities

If you are a student with a disability and believe you will need accommodations for this class, it is your responsibility to contact Student Disability Services at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Disability Services as soon as possible. Please note that accommodations are not retroactive, and that accommodations based upon disability cannot be provided until you have presented your instructor with an accommodation letter from Student Disability Services. Your cooperation is appreciated.

Academic Honesty

The University adheres to a strict policy regarding cheating and plagiarism. These activities will not be tolerated in this class. Become familiar with the policy (http://www.sa.sdsu.edu/srr/conduct1.html). Any cheating or plagiarism will result in failing this class and a disciplinary review by Student Affairs.

Examples of Plagiarism include but are not limited to:

- Using sources verbatim or paraphrasing without giving proper attribution (this can include phrases, sentences, paragraphs and/or pages of work)
- Copying and pasting work from an online or offline source directly and calling it your own
- Using information you find from an online or offline source without giving the author credit
- Replacing words or phrases from another source and inserting your own words or phrases
- Submitting a piece of work you did for one class to another class

If you have questions on what is plagiarism, please consult the policy (http://www.sa.sdsu.edu/srr/conduct1.html) and this helpful guide from the Library:(http://infodome.sdsu.edu/infolit/exploratorium/Standard_5/plagiarism.pdf)

Extra help and tips for Success

Help is available in a variety of forms.

- Work with your classmates on difficult material.
- Utilize office hours.
- Take advantage of the optional reading. The instructor can direct the student to a specific book chapter to help with a certain concept.

10 Musts to get a good grade:

- Attend all lectures.
- Read optional material, prior knowledge will help you become engaged in lecture and better comprehend material.
- Write questions down, and attend office hours.
- Take class projects serious (worth more than tests or presentation).
- Discuss concepts with classmates, or study partner. Practice your presentation in front of your classmates prior to presentation day.
- Do not fall behind.
- Try to see the big picture. NMR is extremely complex. You will not grasp all of it.
- Be curious. Always ask why? Questions are welcome.
- Focus on understanding concepts, not memorization.
- Start early on class projects and presentation. It takes considerable time and effort to write a good report and/or give a good presentation.
- Remember the end goal is to learn practical NMR and how you can apply it to your research interests.