CHE 522

STRUCTURE DETERMINATION IN ORGANIC AND MEDICINAL CHEMISTRY

Course Syllabus

Spring 2018

INSTRUCTOR:	JAVID RZAYEV
OFFICE LOCATION:	NSC 826
OFFICE HOURS:	Wednesday 3-5 pm or by appointment
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CLASS HOURS:	Tu Thu 9:30-10:50am
CLASS LOCATION:	Hoch 114

Spectroscopic techniques are invaluable tools for the structural characterization of organic compounds. This course will provide students with fundamental and practical knowledge on using nuclear magnetic resonance (NMR), infrared (IR) and ultraviolet (UV) spectroscopy and mass spectrometry techniques. After a brief introduction into the theory behind these techniques, the majority of the course will focus on developing data interpretation and problem solving skills. A large portion of the course will be devoted to utilizing 1D and 2D ^{1}H and ^{13}C NMR spectroscopy methods for structure determination of organic compounds. Students will learn how to choose a particular characterization method, design proper experiments, and analyze and interpret the obtained spectra.

TEXTBOOK (not required):

- Crews, Rodriguez and Jaspars, *Organic Structure Analysis*, Oxford University Press, 2nd ed., 2010.

OTHER HELPFUL BOOKS:

- Prefsch et al., *Structure Determination of Organic Compounds*, Springer, 2000.
  A good reference book containing tables of spectral data.
- Lambert et al., *Organic Structural Spectroscopy*, Prentice Hall, 2001.
  Introductory text on spectroscopic techniques for organic structure determination.
- Friebolin, H. *Basic One- and Two-Dimensional NMR Spectroscopy*, 5th Ed., Wiley-VCH, 2011.

COURSE OUTLINE:

- Introduction to organic structure characterization
- Infrared Spectroscopy (brief review)
- Ultraviolet Spectroscopy (brief review)
- Introduction to Nuclear Magnetic Resonance
- Interpretation and use of ^{1}H and ^{13}C chemical shifts
- Interpretation and use of ^{1}H and ^{13}C coupling constants
- Problem solving approaches
- Multiple-pulse and multidimensional NMR techniques
- Advanced problem solving

Exam Schedule

Homework	15%
Quizzes	15%
Midterm I (March 6)	20%
Midterm II (April 24)	20%
Final (May 17)	30%

Learning Outcomes	Assessment Tools
Identify organic functional groups from IR spectra	Midterm 1, Homework 1
Understand the basic of UV spectroscopy and its use in characterization of organic compounds	Midterm 1, Homework 2
Understand the fundamentals of NMR spectroscopy	Midterm 1
Use chemical shifts to identify basic organic structures	Midterm 1, Homework 4
Use spin-spin couplings to interpret more complex NMR spectra	Midterm 2, Homework 5-7
Understand spin-spin and spin-lattice relaxation	Midterm 2
Use DEPT, 1D TOCSY and NOE in characterization of complex organic structures	Midterm 2, Homework 8
Understand the basics of 2D NMR techniques	Final Exam
Use COSY, NOESY, HMQC, HSQC and HMBC in characterization of complex organic structures	Final Exam, Homework 9-10

Note: Additionally, pop quizzes will be used throughout the course to aid in assessing student learning.

The Course: This course will be focused on problem solving. After brief overview of the fundamental concepts, the course will emphasize learning via solving real-life spectroscopic problems. All exams will be open-book, open-notes. You will be responsible for everything covered in class during lectures plus additional reading material. You will benefit from developing a systematic approach to learning the material in this class. The following should be essential elements of any study plan:

1) Regular attendance at lectures.
2) Reviewing and expanding upon your notes as soon as possible after each lecture.
3) Solving as many problems as possible. Practice, practice, practice!

Courtesy: Please be considerate to others during lectures. The use of cell phones (including text messaging) is strictly prohibited during lectures. Please do not disturb others by loud talking, noises and inappropriate behavior. The attendance at lectures will greatly benefit you if you can concentrate and pay full attention to the instructor. However, the attendance is not mandatory. If you feel like taking a nap, please find another room to do so.

Grading: Errors in the grading of examinations should be presented directly to me within one week after the return of the examination papers to class. No grades will be changed after this time. If you want to have your exam regarded, then return it to me along with a note explaining the nature of the error in grading. I reserve the right to regrade your whole exam even if you found an error only in one of the questions.

Missed examinations: Do not miss the exams. Only students with a documented excused absence which is in conformance with the University guidelines for excused absences will be granted a make up exam. Make up exams will cover the same subjects, will be comparable in difficulty, and will be composed of different questions than the missed midterm examination. If proper excuse documentation is provided, every student is eligible for only one make up exam.

Letter grade assignment: The letter grade will be determined from the results of two midterm examinations, the final examination and homework assignments based on the average performance of the class (curve). The last day to "resign" the course (receive grade "R") is April 20. After this time, I am required to assign you a letter grade for your work. For more details, check the Academic Calendar.

Cheating: Cheating is an insidious practice. Your grade is assigned by measuring your performance against the average performance of others in this class. Cheating raises the class average for the benefit of those who cheat, and to the detriment of honest students. Cheaters who are caught in the act will receive zero for the examination. If second academic dishonesty is committed, the student will automatically fail the class.

CHE 522 Course website on UBLearns: The URL for this site is http://ublearns.buffalo.edu/. Syllabus, copies of old examinations, grade distributions and occasional announcements will be posted on this site. Please check the site regularly for class materials.

Accessibility: We appreciate hearing from anyone in this class who has any special needs, and together we can work out the best possible arrangements for you to succeed. Please see me after class, during my office hours, or by appointment as soon as possible.
If you require classroom or testing accommodations due to a disability, please contact Accessibility Resources, located at 25 Capen Hall. AR can be reached by phone at (716) 645-2608 or by email at stu-accessibility@buffalo.edu. Please inform me as soon as possible about your needs so that we can coordinate your accommodations. Accommodations need to be made well in advance, so please do not wait until right before an exam.