Chemistry 635
Spectroscopic Identification of Organic Molecules
Spring 2011

Meetings: MW 6:00-7:15 pm **Location**: Faraday West 201

Instructor: Dr. Dmitry Kadnikov
E-mail: dkadnikov@niu.edu, please include **Chem635** in the subject
Office: Faraday Hall 343 (FR 343)
Office Hours: by appointment; also, if there is an interest, after three or four weeks of classes, we could set up a regular time for a weekly problem solving session
Blackboard: Blackboard will be used to post grades, announcements, keys to quizzes and exams, and all other course related materials

Course Objectives

The main goal of the course is to develop skills necessary to determine a two-dimensional structure of an average medium-size organic molecule from the spectroscopic data. To achieve this goal, you will need to spend a lot of time (much more time than you will spend actually reading the textbook!) solving problems on your own, since experience is the only way to truly learn all the nuances and subtleties and to master the technique. The second but equally important goal is to provide a theoretical background on most important spectroscopic techniques, especially on nuclear magnetic resonance (NMR), to give you a better understanding of the nature of the data collected, to allow you to conduct experiments in a more intelligent fashion, and to identify appropriate experiments necessary to solve more complicated structural problems or to use these spectroscopic methods in other experiments.

Textbook:

Organic Structure Analysis, 2nd Ed. by Philip Crews, Jaime Rodríguez, and Marcel Jaspars (ISBN 0-19-533604-7)

Strongly recommended:

Organic Spectroscopic Structure Determination by Douglas F. Taber (ISBN 978-0-19-531470-0)

Optional:

Basis One- and Two-Dimensional NMR Spectroscopy by Horst Friebolin (ISBN 3-527-31233-1)

Additional literature:

Spectrometric Identification of Organic Compounds 7th Ed. by Robert M. Silverstein, Francis X. Webster, and David Kiemle (ISBN 0-471-39362-2)

Very good as a reference book containing lots of useful information in Tables, some of which are reproduced in Taber (see above), therefore even older editions are useful

Structure Determination of Organic Compounds: Tables of Spectral Data by E. Pretsch, P. Büchmann, and C. Alffolter (ISBN 3540678158)

Not a textbook, but a huge compendium of chemical shifts and coupling constant data for both ^{1}H and ^{13}C NMR. The upcoming editions will contain expanded chapters on ^{19}F, ^{31}P, and ^{29}Si NMR, but any edition contains enough data to be worth the money. And it is cheap: it is a paperback!

NMR Spectroscopy 2nd Ed. By Harald Günther (ISBN 0-471-95201-X)

A slightly more advanced text than Friebolin, but covers all topics we will cover in the course

High-Resolution NMR Techniques in Organic Chemistry by T. D. W. Claridge (ISBN 0080548180)

Modern incarnation of the classic text by Andrew Derome (which is still a great read if you can find it second-hand, ISBN 0080325130), this is an advanced text, presenting NMR using vector notation. You will not find here any information on chemical shifts and coupling constants, but it will provide all you need to know about multi-pulse and multi-dimensional experiments.

Modern NMR Spectroscopy by Jeremy K. M. Sanders and Brian K. Hunter (ISBN 0198555679)

Very similar in organization, approach, and material covered to the Derome and Claridge's books

Infrared Absorption Spectroscopy: Practical by Koji Nakanishi

This one is a classic, pretty much everything you want (and much more than you really need) to know about IR. Unfortunately, it is out of print.

Interpretation of Mass Spectra 4th Ed by Fred W. McLafferty and František Turiček (ISBN 0935702253)

Tentative Course Outline

Below is an approximate outline of topics to be covered as well as appropriate readings from the main textbook (CRJ), as well as the supplementary NMR text (FR). Significant amount of class time will be dedicated to problem solving, thus it is hard to anticipate how far we will be able to advance, and how deep will the material be covered.

		Reading
Introduction and Overview of Spectroscopic Methods	2 hrs	CRJ 1
Mass-Spectrometry	7 hrs	CRJ 6, 7, 8
Infrared Spectroscopy	3 hrs	CRJ 9
Nuclear Magnetic Resonance Spectroscopy		
Fundamentals of the NMR Experiment	2 hrs	CRJ 2.1-2.4, FR 1.1-1.5
Overview of ^{1}H and ^{13}C NMR Spectroscopy	3 hrs	CRJ 2.5-2.10, 3.1-3.4, 4.1-4.2, FR 1.6
Symmetry and Topicity	2 hrs	CRJ 3.5, FR 2.4
Chemical Shifts	2 hrs	CRJ 3.6, FR 2, 6
Spin Systems and Spin Coupling	4 hrs	CRJ 4.3-4.9, FR 3, 5
Introduction to NMR Vector Notation	1 hr	CRJ 5.2, FR 8.2
Complex Pulse Sequences	3 hrs	CRJ 5.2-5.3, FR 8.3-8.8
Two-Dimensional NMR	3 hrs	CRJ 5.4-5.9, FR 9
Nuclear Overhauser Effect	1 hr	CRJ 4.10, FR 10
Additional aspects (relaxation and dynamics)	2 hrs	FR 7, 11
Optical Spectroscopy (ultraviolet, chiral dichroism)	2 hrs	CRJ 10

Grading:	8 quizzes at 10 pts each	= 80 pts
	2 exams at 30 pts each	= 60 pts
	5 home-work sets at 2 pts each	= 10 pts
	Final Exam	= 50 pts
	Total	**= 200 pts**

Starting with the week 6, a quiz will be given during the last third of each Wednesday class (total of eight). Each quiz will consist of one problem on the identification of a 2D structure of an organic molecule from spectroscopic data, which will usually consist of the MS, IR, ^{1}H and ^{13}C NMR spectra. In addition there will be **two midterm** in-class **exams**, on **Wednesday, March 9** and **Wednesday, April 20**. The exams will contain a one or two structure identification problems, worth 10 pts each, and several short answer questions on the material covered in lectures. The **final exam** (which is officially scheduled for **Monday, May 9, 6 – 7:50 pm**, but could be rescheduled by class consensus) will consist of two or three structure identification problems and several short answer questions. All exams and quizzes will be open notes and open book, however, you will not be allowed to use books, which are essentially the lists of organic compounds, such as, for example, an Aldrich catalog or a Dictionary of Organic Compounds. Five take-home problem sets will also be distributed throughout the semester, and you will generally have a week to complete them. You could work in groups, but each work will be graded individually. You will have to answer correctly more than 80% of the questions to receive 2 pts for the problems set, more than 65% to get 1.5 pts, and more than 50 and 30% to receive 1 and 0.5 pts, respectively.