Chemistry 4361/8361 Interpretation of Organic Spectra

Fall 2016 MWF 9:05 am – 9:55 am 231 Smith

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Find class website under http://www.chem.umn.edu/class/

Book E. Pretsch, P. Buhlmann & C. Affolter, Structure Determination of Organic Compounds: Tables of Spectral Data, 4th ed., Springer-Verlag, New York 2009, **highly recommended**.

Course Summary:

This course is intended to be a practical introduction to using spectral tools to elucidate the structures of molecules. In this class we will discuss mainly nuclear magnetic resonance (NMR) spectrometry and mass spectrometry (MS), and to a lesser extent infrared (IR) and ultraviolet-visible (UV-vis) spectroscopy. The class will be focused on determining the structures of organic molecules, but also of some biological, organometallic, and inorganic molecules as well. The class is very much intended to give students the tools they need to determine structures in a research setting. Rather than reading or memorizing, most of your time in this course will be spent solving spectral problems; many of these problems come from current research at the University of Minnesota. If you are not presently doing research involving molecules, or you don't see yourself solving molecular structures for a living in the near future, you will probably not get very much out of this class. On the other hand, if you do or plan to do research involving organic molecules, this class will be extremely useful for you.

Materials on Reserve (available through Walter Library Reserve unless noted.)

P. Crews, J. Rodriguez, M. Jaspars, Organic Structure Analysis (Oxford University Press, New York, 1998).

J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks, Organic Structural Spectroscopy (Prentice-Hall, Upper Saddle River, NJ, 1998). A similar text to Crews. Good source of problems to solve, but no answer key.

E. Breitmaier, Structure Elucidation by NMR in Organic Chemistry: A Practical Guide (Wiley, New York, 2002). Great source of complex NMR problems, with answers.

T. D. W. Claridge, High-Resolution NMR Techniques in Organic Chemistry (Second Edition) (Elsevier, Oxford, 2009). Detailed text on NMR methods. Has a better description of advanced NMR experiments than Crews or Lambert. Available free online through the library.

S. Berger, S. Braun, 200 and More NMR Experiments (Wiley, New York, 2004). A resource with many advanced NMR experiments as well as descriptions of how to run the experiments and pulse sequences.

J. C. Hollerton, S. A. Richards, Essential Practical NMR for Organic Chemistry (Wiley, West Sussex, UK, 2011). This is an excellent resource for practical NMR, from solvent effects to processing spectra. Only available online through the library. (Not downloadable)

E. de Hoffmann, V. Stroobant, Mass Spectrometry: Principles and Applications (Wiley, New York, 1999). Excellent text on methods and interpretation in mass spectrometry.

F. W. McLafferty, F. Turecek, Interpretation of Mass Spectra (University Science Books, Mill Valley, CA, 1993). Classic text on ion abundance and radical fragmentation in mass spectrometry. However, the book has not been updated in quite a while, and doesn't have as much information about modern MS methods. Available online through the library.

D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy (Cengage Learning, Stamford, CT, 2015). A general overview of a number of types of instrumental analysis like IR, UV-Vis, and NMR spectroscopy, as well as mass spectrometry. Also a good source of practice problems.

Grading:

	4361	**8361**
Best 3 of 4 tests at 25% each	75%	75%
Problem sets	25%	10%
Project	–	15%

Four 50-min midterm exams are scheduled on October 7, October 31, November 23, and December 14.

Exams will be open book and open note; you may bring any materials you see fit to exams. However, student cooperation (including sharing materials or notes) during exams is prohibited. You may be excused from taking an exam due to jury duty, subpoenas, military service, religious holidays, and participation in school sports events only if the instructor is notified two weeks in advance. You may also be excused in case of illness (as verified by a doctor's note) or death in the immediate family (be prepared to verify), provided the instructor is notified within 24 hours of the exam.

Problem sets will be handed out in class more or less weekly and will be due the following week at the beginning of class (no late submissions accepted). The problem sets will be discussed in the following discussion section. Problem sets will primarily be graded on effort, and intelligent attempts to answer all problems will receive full credit. Working together on problems is highly encouraged, but you should submit your own solutions.

Labs will be conducted in the Chemistry Department Spectroscopy Facility in 193 Kolthoff. Labs are available and required only for students enrolled in Chem 8361. Detailed descriptions of the required labs will be available on the class website. Instructions for writing up each lab are in the lab instructions. Total credit for all lab write-ups will sum to 150 points.

Policy on "I" Grade: Departmental policy is that a student may request an Incomplete grade only when(a) he or she has a University-sanctioned excuse for missing the final exam and (b) he

or she is passing the course based on all other graded components. Assignment of an I requires that the instructor and student sign a contract, available in the Departmental undergraduate office, stipulating the procedure by which the I grade will be made up (e.g., taking a final exam from another instructor in the next semester). Failure to successfully complete the procedure outlined in the contract will result in the I being administratively changed by the University Registrar to an F or N (depending on the grade base) one calendar year from the end of the semester for which the I grade was granted.

Scholastic Dishonesty: "Scholastic dishonesty is any act that violates the rights of another student with respect to academic work or that involves misrepresentation of a student's own work. Scholastic dishonesty includes (but is not limited to cheating on assignments or examinations; plagiarizing (misrepresenting as one's own work done by another); submitting the same or substantially similar papers for more than one course without consent of all instructors concerned; depriving another of necessary course materials; sabotaging another's work." – *Classroom Grading and Examination Procedures, College of Liberal Arts*.

If a student is guilty of scholastic dishonesty, they will receive no credit, that is, a "0" for the work involved or an "F" for the course, and the incident will be reported to the Scholastic Conduct Committee of the College in which the student is enrolled, resulting in a letter to be included in their file.

Tentative schedule for Chem 4361/8361 – Fall 2016

Date	Lecture	Topic
9/7	1	NMR: Basic concepts
9/9	2	NMR: Basic concepts
9/12	3	NMR: Basic concepts
9/14	4	NMR: Basic concepts
9/16	5	In-class problems index of H deficiency, rule of 13
9/19	6	NMR spectral patterns
9/21	7	Intro to NMR instrumentation in Chemistry by Dr. Letitia Yao, NMR Facility Director
9/23	8	In-class problems
9/26	9	NMR spectral patterns
9/28	10	Intro to MS instrumentation in Chemistry by Dr. Joseph Dalluge, MS Facility Director
9/30	11	In-class problems
10/3	12	Spin-spin coupling
10/5	13	Spin-spin coupling
10/7	Exam 1	
10/10	18	Mass spectrometry
10/12	19	Mass spectrometry
10/14	20	In-class problems
10/17	21	Mass spectrometry
10/19	22	2D NMR methods
10/21	23	In-class problems
10/24	24	2D NMR methods
10/26	25	2D NMR methods
10/28	26	In-class problems
10/31	Exam 2	
11/2	27	2D NMR: HMQC, HSQC & HMBC
11/4	28	In-class problems

11/7	29	2D NMR: INADEQUATE
11/9	30	Stereochemistry: nOe & NOESY/ROESY
11/11	31	In-class problems
11/14	32	Stereochemistry: Acetonides & Quantitative NMR
11/16	33	
11/18	34	In-class problems
11/21	35	Organometallic complexes
11/23	Exam 3	
11/25		Thanksgiving break
11/28	35	
11/30	37	
12/2	38	In-class problems
12/5	39	Putting It All Together
12/7	40	Putting It All Together
12/9		In-class problems
12/12		
12/14	Exam 4	