

**Chemistry 425/395**  
**Spectroscopy and Structural Elucidation**

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Spring 2012  
MW 5:30-6:50, FH 105

This course will introduce the use of spectroscopy for the elucidation of organic structures. The methods will include IR spectroscopy, UV-Vis spectroscopy, Mass spectrometry, NMR techniques ( $^1\text{H}$ ,  $^{13}\text{C}$ , and 2D), X-ray, and related computational techniques. The course will focus on the application of these methods in solving structures of organic molecules, with some instrument theory, some history, method development, and pertinent websites and books.

**Course Information:**

1. Grading:	Midterm Exam 1	100pts	22.2%
	Midterm Exam 2	100pts	22.2%
	Final Exam	150pts	33.3%
	Problem Sets #1-3	75pts	16.7%
	Presentation	25pts	5.6%
	Total	450pts	100%

2. **Office Hours:** MW 3:30- to before class in FH 212; other times, by appointment.

3. **Textbook** Lambert, Shurve, Lightner, Cooks, "Organic Structural Spectroscopy 2/E", Prentice-Hall, Upper Saddle River, NJ, 2011. This text is the only source material permitted during exams.

**4. Other General References Spectroscopy Texts:**

P. Crews, Rodriguez, Jaspars, "Organic Structure Analysis 2<sup>nd</sup> Ed," Oxford University Press, 2009.  
J. Lambert, Shurve, Lightner, Cooks, "Organic Structural Spectroscopy", Prentice-Hall, Upper Saddle River, NJ, 1998.  
Silverstein, Webster, Kiemie "Spectroscopic Identification of Organic Compounds, 6<sup>th</sup> Ed. Wiley 2005.  
Pavia, Lampman, Kriz, & Vyvyan "Introduction to Spectroscopy 4<sup>th</sup> Ed" Saunders College Pub, 2009.  
Williams and Fleming, "Spectroscopic Methods in Organic Chemistry" 5<sup>th</sup> Ed. McGraw Hill, 1995  
Field, Sternhell, Kalman, Organic Structures from Spectra 4<sup>th</sup> Ed., Wiley, 2008

**5. Other Spectroscopy Texts:**

Breitmaier, "Structure Elucidation by NMR in Organic Chemistry"  
Derome, "Modern NMR Techniques for Chemistry Research" Pergamon, 1987.  
Duddeck, "Structure Elucidation by Modern NMR"  
Jacobsen, "NMR Spectroscopy Explained" Wiley, 2007.  
Kemp, "Organic Spectroscopy" 3<sup>rd</sup> Ed. Freeman, NY 1991.  
Macomber, "A Complete Introduction to Modern NMR Spectroscopy," Wiley, 1998.  
McLafferty & Turecek, "Interp. of Mass Spectra" 4<sup>th</sup> Ed", University Science Books, 1993.  
Nelson, J. H., "NMR Spectroscopy" Prentice Hall, NJ, 2003.  
Pretsch, Buhlmann, Affolter, "Structure Det. of Organic Compds 3<sup>rd</sup> Ed." Springer, 2000  
Wehrli, Marchand, & Wehrli "Interp. of Carbon-13 NMR Spectra" 2<sup>nd</sup> Ed, Wiley, 1988.

**6. Computational Suites**

ACD Labs, Hyperchem, ChemDraw Professional  
ChemWindows-Spectroscopy & newer versions