Chemistry 425/395 (Draft)
Spectroscopy and Structural Elucidation

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Spring 2013
MW 4:00-5:30, 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}H, ^{13}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 SpectroscopyTexts:**
   P. Crews, Rodriguez, Jaspars,"Organic Structure Analysis 2nd Ed," OxfordUniversity.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, 6th Ed. Wiley 2005.
   Pavia, Lampman, Kriz, &Vyvyan "Introduction to Spectroscopy 4th Ed" Saunders College Pub, 2009.
   Williams and Fleming, "Spectroscopic Methods in Organic Chemistry" 5thEd.McGrawHill, 1995
   Field, Sternhell, Kalman, Organic Structures from Spectra 4th 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" 3rd Ed. Freeman, NY 1991.
   Macomber, "A Complete Introduction to Modern NMR Spectroscopy," Wiley, 1998.
   McLafferty & Turecek, "Interp. of Mass Spectra" 4th Ed", University Science Books, 1993.
   Nelson, J. H., "NMR Spectroscopy" Prentice Hall, NJ, 2003.
   Pretsch, Buhlmann, Affolter, "Structure Det. of Organic Compds 3rd Ed." Springer, 2000
   Wehrli, Marchand,& Wehrli "Interp. of Carbon-13 NMR Spectra" 2nd Ed, Wiley, 1988.

6. **Computational Suites**
   ACD Labs, Hyperchem, ChemDraw Professional
   ChemWindows-Spectroscopy & newer versions

7. Schedule

Spectroscopy Chemistry 425-/395, Spring 2013
Lecture Outline
(Tentative)

Date	Chap	Topic	Tentative Lecturers
Jan 14	1	Background Info: Introduction; Analysis or Separation of mixtures; Purification.	**DC**
Jan 23	2/3	^{1}H NMR: History, definitions, theory, chemical shifts, assignments, integration	**DC**
Jan 25	2/3	^{13}C NMR: Theory, Chemical shifts, Coupling/Decoupling, Assignments,	**DC**
Jan 30	4	Coupling constants, signs, classification of spin systems, Problems	**DC**
Feb 1	2	NMR: relaxation (T_1 & T_2), simulations, solvent effects, Problems	**DC**
Feb 6		NMR: Computations, Simulations, Problem Solving **Problem Set 1**	**JB**
Feb 8	5	^{13}C NMR: APT, Relaxation, INEPT, DEPT techniques	**DC**
Feb 13	11	IR: Theory of Dispersive & FTIR, characteristic absorptions, symmetry	**DC**
Feb 15	12	IR: absorptions cont'd, problem solving, databases, Raman, AFM,SEM	**DC**
Feb 20	13	UV-Vis: Theory, excited states, transitions, notation, (**Prob Set 1 due**.)	**DC**
Feb 22	14	UV-Vis:, chromophores Woodward-Fieser Rules, Charge Transfer, CD, ORD	**DC**
Feb 27	Book	Problem Solving combining NMR, IR, and UV/Vis **Problem Set 2** Websites?	**DC**
Feb 29		**Midterm Exam #1**	
Mar 5-7		*Mid-semester break* **ENJOY!**	
Mar 12	6	2DNMR: Intro, Theory, Correlation w coupling COSY, TOCSY **Prob Set #2 due**	**DC**
Mar 14	6	2D NMR: Techniques, indirect detection, HMQC, Acronyms, & Applications	**DC**
Mar 19	6	2D NMR: Problem solving	**DC**
Mar 21		More NMR: (catchup if needed), VT, Heteroatoms, CIDNP,	**DC**
Mar 26		**ACS** X-Ray Diffraction	**DL**
Mar 28		**ACS Midterm Exam #2**	
Apr 2	7	MS: Theory, Instrumentation, and Sample Preparation	**DC**
Apr 4	8	MS: Ion activation and Fragmentation	**DC**
Apr 5-8		Easter Break	
Apr 9	9	MS Structural Analysis (Class is after 4:15.)	
Apr 11	10	MS: Quantitative Apps. and problem solving	**DC**
Apr 16	15	Larger Molecules & Other Techniques	
Apr 18		*Student Presentations*	
Apr 23		*Student Presentations*	
Apr 25		*Student Presentations*	
Apr 30		Review Day & Problem Solving practice	
May 2 ?		**Final Exam w Textbook**	

Lecturers: J.Babler, D.Liu,

Topics Not Covered: NIR, CD, ORD, 3 & 4 D-NMR, EPR, etc

Prob Set 1: 10 spectra from AIST (see below)
Prob Set 2: 5 from AIST + others
Prob Set 3: 5 from anywhere

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8. Spectroscopy Websites that may be useful (January 2012). Using Google: "Spectroscopy" gave 3.4 x 10^7 hits; "Organic Spectroscopy" gave 1.3 x 10^7 hits; " Organic Spectroscopy Problems" gave 7.9 x 10^6 hits; etc.

Twelve Examples are listed below.

1. *Wikipedia/* ***organic spectroscopy*** "Spectroscopy," lots of info and branches (NMR. IR, Woodward Rules).

2. spectroscopyNOW.com - spectroscopy and spectrometry portal (John Wiley & Sons)
Spectroscopy portal addressing mass spectrometry, NMR, MRI, x-ray, atomic, Raman, IR, UV, proteomics and chemometrics and informatics techniques. You can register for info. www.**spectroscopy**now.com

3. WebSpectra - Problems in NMR and IR Spectroscopy
More NMR practice problems and a great outline of spectral assignments methods.
www.chem.ucla.edu/~webspectra/ - 21k. mainly ^{1}H, ^{13}C, and IR only a few others.

4. Organic Chemistry On Line A good introduction to modern NMR **spectroscopy**. **...** A nice collection of problems using all the **spectroscopy** methods discussed here.
www.cem.msu.edu/~reusch/VirtualText/Spectrpy/spectro.htm -

5. http://www.cis.rit.edu/htbooks/nmr/ {exceptional exposition on NMR}

6. NMR Spectroscopy - Theory A nice little intro to NMR & IR **spectroscopy** theory.
teaching.shu.ac.uk/hwb/chemistry/tutorials/molspec/nmr1.htm

7. Spectroscopy **Spectroscopic** databases can aid the UK chemist in spectral interpretation and structure elucidation. Searches can be conducted https://cds.dl.ac.uk/cds/help/overview.html
8. Organic Structure Elucidation Workbook **http://www.nd.edu/~smithgrp/structure/workbook.html** **Good** ^{1}H, ^{13}C and MS **Problems** with relative difficulty listed. No answers included.

9. Spectroscopy Problems We have used these **problems** for many years in the **spectroscopy** section of the **organic** chemistry lab and lecture courses. orgchem.colorado.edu/hndbksupport/specttutor/main.html - 6k
Problems include ^{1}H NMR and IR data with answers and some interpretation.

10. CHP - ***Spectroscopy*** ***Spectroscopy*** **is the use of the absorption, emission, or scattering of electromagnetic radiation by matter to qualitatively or quantitatively study..Not only organic ...**
www.files.chem.vt.edu/chem-ed/spec/spectros.html **- Cached - Similar**

11. http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng SDBS from AIST of Japan with combined spectra. http://www.aist.go.jp/RIODB/SDBS/cgi-bin/cre_index.cgi (Japanese version) A recent announcement says service depends on availability of electricity after last year's earthquake.

12. *www.ups.edu/faculty/hanson/chemwebsites/**organic**websites.htm* A list of organic related sites. However, the sites listed first and fourth did not work for me as of Jan 2012.