

Course Syllabus

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Molecular Structure/Spectroscopy of Organic Compounds (CHEM 7310)

Instructor: Prof. Brad Davidson

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Meeting Time/Place: TBD

Office Hours: Anytime

Prerequisites: CHEM 6300

Materials:

- "Spectroscopic Identification of Organic Compounds," R.M. Silverstein, R.X. Webster, D.J. Kiemle, and D.L. Bryce, 8th Edition, 2015.
- "Structure Determination of Organic Compounds: Tables of Spectral Data," E. Pretsch, P. Buhlmann, and M. Badertscher; 4th Edition, 2009. (Optional)
- "High-Resolution NMR Techniques in Organic Chemistry," T. D. W. Claridge, 2nd Edition, 2009. (Optional)

Course Goals: To gain experience with modern methods available for the determination of two- and three-dimensional structures of organic compounds. Instrumental techniques, including NMR, MS, IR, and UV will be stressed, but some chemical methods will be included. The application of individual techniques and the interpretation of data will be emphasized along with a minimal amount of theory.

Grading:

Problem sets (6 x 50 pt)	300
Presentation	50
Midterm exams (2 x 100 pt)	200
Take-home final	150
Total Points	700

Useful Links:

Electromagnetic Radiation:

[Electromagnetic Spectrum Figure](http://www.lbl.gov/MicroWorlds/ALSTool/EMSpec/EMSpec2.html) (<http://www.lbl.gov/MicroWorlds/ALSTool/EMSpec/EMSpec2.html>)

Mass Spectrometry:

[Tutorials](http://www.chem.arizona.edu/massspec/) (<http://www.chem.arizona.edu/massspec/>)

[Isotope Clusters](http://www.colby.edu/chemistry/NMR/IsoClus.html) (<http://www.colby.edu/chemistry/NMR/IsoClus.html>)

[Isotope and Molecular Weight Calculations](http://www-jmg.ch.cam.ac.uk/tools/magnus/MolWeight.html) [\(http://www-jmg.ch.cam.ac.uk/tools/magnus/MolWeight.html\)](http://www-jmg.ch.cam.ac.uk/tools/magnus/MolWeight.html)

[Molecular Formulas from HRMS data](http://www-jmg.ch.cam.ac.uk/tools/magnus/EadFormW.html) [\(http://www-jmg.ch.cam.ac.uk/tools/magnus/EadFormW.html\)](http://www-jmg.ch.cam.ac.uk/tools/magnus/EadFormW.html)

IR Spectroscopy:

NMR Spectroscopy:

[WebSpectra](http://www.chem.ucla.edu/~webspectra/) [\(http://www.chem.ucla.edu/~webspectra/\)](http://www.chem.ucla.edu/~webspectra/)

[Conformational analysis of natural products](http://www.stenutz.eu/conf/index.html) [\(http://www.stenutz.eu/conf/index.html\)](http://www.stenutz.eu/conf/index.html)

General Spectroscopy:

[MS, IR, UV/Vis, and NMR](http://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/Spectrpy/spectro.htm#intro) [\(http://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/Spectrpy/spectro.htm#intro\)](http://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/Spectrpy/spectro.htm#intro)

[Organic Structure Elucidation Workbook](http://www3.nd.edu/~smithgrp/structure/workbook.html) [\(http://www3.nd.edu/~smithgrp/structure/workbook.html\)](http://www3.nd.edu/~smithgrp/structure/workbook.html)

[NIST Chemistry WebBook](http://webbook.nist.gov/chemistry/) [\(http://webbook.nist.gov/chemistry/\)](http://webbook.nist.gov/chemistry/)

[Database of NMR spectra](http://www.nmrdb.org) [\(http://www.nmrdb.org\)](http://www.nmrdb.org)

Comments:

- To become proficient in interpreting spectroscopic data, practice is essential. Organic molecules may include an almost infinite combination of functional groups, only a few of which can be reviewed during this course. Therefore, you will be required to use your imagination and logic to piece together data in attempt to deduce the structures of molecules that are unlike those you have previously seen.
- Teamwork and the use of data tables and textbooks are permissible on problem sets, but the primary literature is off limits. Final answers to be turned in must be written up individually. Problem sets will be due at the beginning of class one week after they have been handed out.
- Mid-term exams will be scheduled for 3 hr during a non-class time, when all are available. They will be open book.
- The final exam will be take-home, and must be completed independently, using any resource other than the primary literature.
- During the last week of the semester, each student will give a 10-15 min presentation on a topic of their choice that is relevant to the course material. Topics should be discussed with the instructor at least 2 weeks in advance.
- Reasonable accommodation will be provided for all persons with disabilities in order to insure equal participation with the program.
- Information concerning dropping classes, academic honesty/honor code, and other academic policies is available in the Schedule of Classes.

Proposed Schedule

Week	Dates	Subject	Reading
1	8/29	Introduction; pre-test; classical structure determination	
		1D NMR Spectroscopy – Proton	
1-3	8/31-9/14	<ul style="list-style-type: none">• Theory• Chemical shift• Spin coupling• Chemical shift equivalence• Nuclear Overhauser effect	Chapt 3

4-5	9/19-9/28	1D NMR Spectroscopy – Carbon <ul style="list-style-type: none"> • Theory • Spin Coupling • Chemical Shift • DEPT 	Chapt 4
6	10/3-10/5	IR Spectroscopy <ul style="list-style-type: none"> • Theory • Functional group absorptions 	Chapt 2
7	10/10-10/12	UV/Vis Spectroscopy <ul style="list-style-type: none"> • Theory • Lambert-Beer law • lambda max predictions 	Handout
		Exam 1 (date and time TBD)	
8-9	10/17-10/26	Mass spectrometry <ul style="list-style-type: none"> • Theory <ul style="list-style-type: none"> – ionization techniques – mass analyzers • Interpretation <ul style="list-style-type: none"> – molecular ion – fragmentation 	Chapt 1
10-11	10/31-11/9	Advanced NMR – Correlation Spectroscopy <ul style="list-style-type: none"> • Theory <ul style="list-style-type: none"> – rotating frame – pulse sequences – experimental considerations • Homonuclear • Heteronuclear • Applications/examples 	Chapt 5
		Exam 2 (date and time TBD)	
12	11/14-11/16	NMR of Other Nuclei	Chapt 6
13-14	11/21-11/30	Stereochemistry <ul style="list-style-type: none"> • Relative <ul style="list-style-type: none"> – <i>J</i>-coupling – nuclear Overhauser effect • Absolute <ul style="list-style-type: none"> – NMR methods – optical methods 	Handouts
15	12/5-12/7	Presentations	
16		FINAL (Take-home; pick-up 12/12, due 12/16, 5:00 PM)	

Assignments Summary:

Date	Details
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