

## Course Syllabus

# Molecular Structure/Spectroscopy of Organic Compounds (CHEM 7310)

## Instructor Contact Information:

Prof. Brad Davidson

Office: Widtsoe 341

Phone: 797-1628

e-mail: [brad.davidson@usu.edu](mailto:brad.davidson@usu.edu) (<mailto:brad.davidson@usu.edu>)

Meeting Time/Place: T & Th, 9:30-10:45 AM; MCL 151

Office Hours: Anytime

Prerequisites: CHEM 6300

## Course Description:

Modern methods of predicting and determining molecular structure of organic compounds using advanced computational and spectroscopic tools.

## 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.

## Course Materials:

- "Spectroscopic Identification of Organic Compounds," R.M. Silverstein, R.X. Webster, D.J. Kiemle, and D.L Bryce, 8<sup>th</sup> 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)

## Grading:

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

## 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)

[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)

### IR Spectroscopy:

### NMR Spectroscopy:

[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)

### 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)

[Organic Structure Elucidation Workbook](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/)

## 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 an non-class time, when all are available. They will be open book.
- The final exam will be take-home, and must 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	1/8	Introduction; pre-test; classical structure determination	
		1D NMR Spectroscopy – Proton	
1-3	1/10-1/24	<ul style="list-style-type: none"><li>• Theory</li><li>• Chemical shift</li><li>• Spin coupling</li><li>• Chemical shift equivalence</li><li>• Nuclear Overhauser effect</li></ul>	Chapt 3
		1D NMR Spectroscopy – Carbon	
4-5	1/29-2/7	<ul style="list-style-type: none"><li>• Theory</li><li>• Spin Coupling</li><li>• Chemical Shift</li><li>• DEPT</li></ul>	Chapt 4

6	2/12-2/14	IR Spectroscopy <ul style="list-style-type: none"> <li>• Theory</li> <li>• Functional group absorptions</li> </ul>	Chapt 2
7	2/19-2/21	UV/Vis Spectroscopy <ul style="list-style-type: none"> <li>• Theory</li> <li>• Lambert-Beer law</li> <li>• lambda max predictions</li> </ul>	Handout
		<b>Exam 1</b> (date and time TBD)	
8-9	2/26-3/7	Mass spectrometry <ul style="list-style-type: none"> <li>• Theory               <ul style="list-style-type: none"> <li>– ionization techniques</li> <li>– mass analyzers</li> </ul> </li> <li>• Interpretation               <ul style="list-style-type: none"> <li>– molecular ion</li> <li>– fragmentation</li> </ul> </li> </ul>	Chapt 1
	3/11-3/14	SPRING BREAK	
10-11	3/18-3/28	Advanced NMR – Correlation Spectroscopy <ul style="list-style-type: none"> <li>• Theory               <ul style="list-style-type: none"> <li>– rotating frame</li> <li>– pulse sequences</li> <li>– experimental considerations</li> </ul> </li> <li>• Homonuclear</li> <li>• Heteronuclear</li> <li>• Applications/examples</li> </ul>	Chapt 5
		<b>Exam 2</b> (date and time TBD)	
12	4/2-4/4	NMR of Other Nuclei <ul style="list-style-type: none"> <li>• Relative               <ul style="list-style-type: none"> <li>– <i>J</i>-coupling</li> </ul> </li> <li>• Absolute               <ul style="list-style-type: none"> <li>– nuclear Overhauser effect</li> </ul> </li> </ul>	Chapt 6
13-14	4/9-4/16	Stereochemistry <ul style="list-style-type: none"> <li>• Relative               <ul style="list-style-type: none"> <li>– nuclear Overhauser effect</li> </ul> </li> <li>• Absolute               <ul style="list-style-type: none"> <li>– NMR methods</li> <li>– optical methods</li> </ul> </li> </ul>	Handouts
14-15	4/18-4/23	Presentations	
16		<b>FINAL</b> (Take-home; pick-up 4/24, due 4/30, 5:00 PM)	

# University Policies and Procedures:

## Academic Freedom and Professional Responsibilities

Academic freedom is the right to teach, study, discuss, investigate, discover, create, and publish freely. Academic freedom protects the rights of faculty members in teaching and of students in learning. Freedom in research is fundamental to the advancement of truth. Faculty members are entitled to full freedom in teaching, research, and creative activities, subject to the limitations imposed by professional responsibility. Faculty Code Policy #403 further defines academic freedom and professional responsibilities.

## Academic Integrity – "The Honor System"

Each student has the right and duty to pursue his or her academic experience free of dishonesty. The Honor System is designed to establish the higher level of conduct expected and required of all Utah State University students.

The Honor Pledge: To enhance the learning environment at Utah State University and to develop student academic integrity, each student agrees to the following Honor Pledge:

*"I pledge, on my honor, to conduct myself with the foremost level of academic integrity."*

A student who lives by the Honor Pledge is a student who does more than not cheat, falsify, or plagiarize. A student who lives by the Honor Pledge:

- Espouses academic integrity as an underlying and essential principle of the Utah State University community;
- Understands that each act of academic dishonesty devalues every degree that is awarded by this institution; and
- Is a welcomed and valued member of Utah State University.

## Academic Dishonesty:

The instructor of this course will take appropriate actions in response to Academic Dishonesty, as defined the University's Student Code. Acts of academic dishonesty include but are not limited to:

### **Cheating:**

Using, attempting to use, or providing others with any unauthorized assistance in taking quizzes, tests, examinations, or in any other academic exercise or activity will be considered as cheating. Unauthorized assistance includes:

- Working in a group when the instructor has designated that the quiz, test, examination, or any other academic exercise or activity be done "individually;"
- Depending on the aid of sources beyond those authorized by the instructor in writing papers, preparing

reports, solving problems, or carrying out other assignments;

- Substituting for another student, or permitting another student to substitute for oneself, in taking an examination or preparing academic work;
- Acquiring tests or other academic material belonging to a faculty member, staff member, or another student without express permission;
- Continuing to write after time has been called on a quiz, test, examination, or any other academic exercise or activity;
- Submitting substantially the same work for credit in more than one class, except with prior approval of the instructor; or engaging in any form of research fraud.

### **Falsification:**

Altering or fabricating any information or citation in an academic exercise or activity is considered as falsification.

### **Plagiarism:**

Representing, by paraphrase or direct quotation, the published or unpublished work of another person as one's own in any academic exercise or activity without full and clear acknowledgment is plagiarism. It also includes using materials prepared by another person or by an agency engaged in the sale of term papers or other academic materials.

### **Sexual Harassment:**

Sexual harassment is defined by the Affirmative Action/Equal Employment Opportunity Commission as any "unwelcome sexual advances, requests for sexual favors, and other verbal or physical conduct of a sexual nature." If you feel you are a victim of sexual harassment, you may talk to or file a complaint with the Affirmative Action/Equal Employment Opportunity Office located in Old Main, Room 161, or call the AA/EEO Office at (435) 797-1266.

### **Withdrawal Policy and "I" Grade Policy:**

Students are required to complete all courses for which they are registered by the end of the semester. In some cases, a student may be unable to complete all of the coursework because of extenuating circumstances, but not due to poor performance or to retain financial aid. The term 'extenuating' circumstances includes: (1) incapacitating illness which prevents a student from attending classes for a minimum period of two weeks, (2) a death in the immediate family, (3) financial responsibilities requiring a student to alter a work schedule to secure employment, (4) change in work schedule as required by an employer, or (5) other emergencies deemed appropriate by the instructor.

### **Students with Disabilities:**

Students with ADA-documented physical, sensory, emotional or medical impairments may be eligible for reasonable accommodations. Veterans may also be eligible for services. All accommodations are coordinated through the Disability Resource Center (DRC). Please contact the DRC prior to or as early in the semester as possible. Alternate formats for course content are available with advanced notice. Contacting the Disability Resource Center (DRC):

- On Campus: Room 101 of the University Inn
- Phone: 435-797-2444
- [DRC Website](http://www.usu.edu/drc/) [\(http://www.usu.edu/drc/\)](http://www.usu.edu/drc/)

#### Disability related resources for current students:

- [DRC Student Handbook](http://www.usu.edu/drc/currentstudents/handbook/) [\(http://www.usu.edu/drc/currentstudents/handbook/\)](http://www.usu.edu/drc/currentstudents/handbook/)
- [Deaf and Hard of Hearing Student Handbook](http://www.usu.edu/drc/currentstudents/DHHHandbook/) [\(http://www.usu.edu/drc/currentstudents/DHHHandbook/\)](http://www.usu.edu/drc/currentstudents/DHHHandbook/)
- [Disability Related Scholarships](http://www.usu.edu/drc/currentstudents/scholarships/) [\(http://www.usu.edu/drc/currentstudents/scholarships/\)](http://www.usu.edu/drc/currentstudents/scholarships/)
- [Campus Resources](http://www.usu.edu/drc/currentstudents/campusresources/) [\(http://www.usu.edu/drc/currentstudents/campusresources/\)](http://www.usu.edu/drc/currentstudents/campusresources/)
- [Documentation Guidelines](http://www.usu.edu/drc/prospectivestudents/docguide/) [\(http://www.usu.edu/drc/prospectivestudents/docguide/\)](http://www.usu.edu/drc/prospectivestudents/docguide/)
- [Online Resources for Students with Disabilities](http://www.usu.edu/drc/currentstudents/onlineresources/) [\(http://www.usu.edu/drc/currentstudents/onlineresources/\)](http://www.usu.edu/drc/currentstudents/onlineresources/)

#### Diversity Statement:

Regardless of intent, careless or ill-informed remarks can be offensive and hurtful to others and detract from the learning climate. If you feel uncomfortable in a classroom due to offensive language or actions by an instructor or student(s) regarding ethnicity, gender, or sexual orientation, contact:

- [Student Services](http://www.usu.edu/student-services/) [\(http://www.usu.edu/student-services/\)](http://www.usu.edu/student-services/): (435) 797-1712, [studentservices@usu.edu](mailto:studentservices@usu.edu) [\(<mailto:studentservices@usu.edu>\)](mailto:studentservices@usu.edu), TSC 220
- [Student Advocates](http://www.usu.edu/ususa/legal/) [\(http://www.usu.edu/ususa/legal/\)](http://www.usu.edu/ususa/legal/): (435) 797-2912, TSC 340
- [Access and Diversity](http://www.usu.edu/accesscenter/) [\(http://www.usu.edu/accesscenter/\)](http://www.usu.edu/accesscenter/): (435) 797-1728, [access@usu.edu](mailto:access@usu.edu) [\(<mailto:access@usu.edu>\)](mailto:access@usu.edu), TSC 315
- [Multicultural Programs](http://www.usu.edu/accesscenter/multiculture/) [\(http://www.usu.edu/accesscenter/multiculture/\)](http://www.usu.edu/accesscenter/multiculture/): (435) 797-1728, TSC 315
- [LGBTQA Programs](http://www.usu.edu/accesscenter/lgbtqa/) [\(http://www.usu.edu/accesscenter/lgbtqa/\)](http://www.usu.edu/accesscenter/lgbtqa/): (435) 797-GAYS, TSC 314
- [Provost's Office Diversity Resources](http://www.usu.edu/provost/faculty/diversity/) [\(http://www.usu.edu/provost/faculty/diversity/\)](http://www.usu.edu/provost/faculty/diversity/): (435) 797-8176

You can learn about your student rights by visiting:


[The Code of Policies and Procedures for Students at Utah State University](http://www.usu.edu/student-services/student-code/)  
[\(http://www.usu.edu/student-services/student-code/\)](http://www.usu.edu/student-services/student-code/)

## Course Summary:


Date

Details


---

- 
-  [Exam 1 \(https://usu.instructure.com/courses/531657/assignments/2564205\)](https://usu.instructure.com/courses/531657/assignments/2564205)


---

  -  [Exam 2 \(https://usu.instructure.com/courses/531657/assignments/2564206\)](https://usu.instructure.com/courses/531657/assignments/2564206)


---

  -  [Final Exam \(https://usu.instructure.com/courses/531657/assignments/2564207\)](https://usu.instructure.com/courses/531657/assignments/2564207)


---

  -  [Homework1 \(https://usu.instructure.com/courses/531657/assignments/2564208\)](https://usu.instructure.com/courses/531657/assignments/2564208)


---

  -  [Homework2 \(https://usu.instructure.com/courses/531657/assignments/2564209\)](https://usu.instructure.com/courses/531657/assignments/2564209)


---

  -  [Homework3 \(https://usu.instructure.com/courses/531657/assignments/2564210\)](https://usu.instructure.com/courses/531657/assignments/2564210)


---

  -  [Homework4 \(https://usu.instructure.com/courses/531657/assignments/2564211\)](https://usu.instructure.com/courses/531657/assignments/2564211)


---

  -  [Homework5 \(https://usu.instructure.com/courses/531657/assignments/2564212\)](https://usu.instructure.com/courses/531657/assignments/2564212)

---

  -  [Homework6 \(https://usu.instructure.com/courses/531657/assignments/2564213\)](https://usu.instructure.com/courses/531657/assignments/2564213)

---

  -  [Presentation \(https://usu.instructure.com/courses/531657/assignments/2564214\)](https://usu.instructure.com/courses/531657/assignments/2564214)
-