

Course Syllabus

Molecular Structure/Spectroscopy of Organic Compounds (CHEM 7310)

Instructor Contact Information:

Prof. Brad Davidson

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Meeting Time/Place: M, F 12:00-1:15 PM

Office Hours: Upon request

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 Prerequisites:

Coursework prerequisite: CHEM 2320, or equivalent.

Technology: You must have a computer with reliable high speed internet access to complete this course. Late assignments will not be accepted because of unreliable internet access.

- You will need Microsoft Office applications (Word, Power Point, and Excel), Adobe Acrobat, or a PDF viewer to open some of the course materials.
- If you do not have a computer at home with the necessary software or high speed internet access, use the computers available to you on campus.

- Please check your browser at the beginning of each semester and download appropriate software and plugins.

The [Technical Requirements \(https://community.canvaslms.com/docs/DOC-10720-67952720329\)](https://community.canvaslms.com/docs/DOC-10720-67952720329) page identifies the browsers, operating systems, and plugins that work best with Canvas. If you are new to Canvas quickly review the [Canvas Student Orientation](#) materials.

Course 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)

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 \(https://www.cif.iastate.edu/mass-spec/ms-tutorial\)](https://www.cif.iastate.edu/mass-spec/ms-tutorial)

[Online MS Tools \(https://www.sisweb.com/mstools.htm\)](https://www.sisweb.com/mstools.htm)

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

[Molecular Formulas from HRMS data \(https://www.chemcalc.org/mf-finder\)](https://www.chemcalc.org/mf-finder)

IR Spectroscopy:

[IR tutorial](https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm) [_ \(https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm\)](https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm)

NMR Spectroscopy:

[Reich Collection - Notes on NMR](https://organicchemistrydata.org/hansreich/resources/nmr/) [_ \(https://organicchemistrydata.org/hansreich/resources/nmr/\)](https://organicchemistrydata.org/hansreich/resources/nmr/)

[Introductory NMR videos](https://www.youtube.com/playlist?list=PLD14D78BC61685BD7) [_ \(https://www.youtube.com/playlist?list=PLD14D78BC61685BD7\)](https://www.youtube.com/playlist?list=PLD14D78BC61685BD7)

MRI videos ([nuclear spin](https://www.youtube.com/watch?v=IWiAJPjFrFI&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=3) [_ \(https://www.youtube.com/watch?v=IWiAJPjFrFI&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=3\)](https://www.youtube.com/watch?v=IWiAJPjFrFI&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=3), [generating signal](https://www.youtube.com/watch?v=W9EJ2iq0vNM&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=5) [_ \(https://www.youtube.com/watch?v=W9EJ2iq0vNM&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=5\)](https://www.youtube.com/watch?v=W9EJ2iq0vNM&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=5), [T₁ relaxation](https://www.youtube.com/watch?v=NvsM3d4mkTM&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=11) [_ \(https://www.youtube.com/watch?v=NvsM3d4mkTM&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=11\)](https://www.youtube.com/watch?v=NvsM3d4mkTM&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=11), [T₂ and spin-echo](https://www.youtube.com/watch?v=gqgC2XD0Oe8&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=8) [_ \(https://www.youtube.com/watch?v=gqgC2XD0Oe8&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=8\)](https://www.youtube.com/watch?v=gqgC2XD0Oe8&list=PL_iaBDDMPsLdxnrwHbVIEsY6-JZOGnho&index=8).)

[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)

[Questions and Answers in MRI](http://mriquestions.com/index.html) [_ \(http://mriquestions.com/index.html\)](http://mriquestions.com/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)

[Web Spectra](https://webspectra.chem.ucla.edu/) [_ \(https://webspectra.chem.ucla.edu/\)](https://webspectra.chem.ucla.edu/)

[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 and problem sets and exams from past students are off limits. Final answers to be turned in must be written up individually.

- Mid-term exams will be scheduled for 3 hr during a non-class time, when all are available. They will be open text book.
- The final exam will be take-home, and must be completed independently, using any resource other than the primary literature. You will have four days to complete the exam.
- 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		Introduction; pre-test; classical structure determination	
		1D NMR Spectroscopy – Proton	
1-3		<ul style="list-style-type: none"> • Theory • Chemical shift • Spin coupling • Chemical shift equivalence • Nuclear Overhauser effect 	Chapt 3
		1D NMR Spectroscopy – Carbon	
4-5		<ul style="list-style-type: none"> • Theory • Spin Coupling • Chemical Shift • DEPT 	Chapt 4
		IR Spectroscopy	
6		<ul style="list-style-type: none"> • Theory • Functional group absorptions 	Chapt 2
		UV/Vis Spectroscopy	
7		<ul style="list-style-type: none"> • Theory • Lambert-Beer law • lambda max predictions 	Handout
		Exam 1 (date and time TBD)	
8-10		Mass spectrometry	Chapt 1

- Theory
 - ionization techniques
 - mass analyzers
- Interpretation
 - molecular ion
 - fragmentation

Advanced NMR – Correlation Spectroscopy

- | | | |
|-------|---|---------|
| 11-12 | <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)

- | | | |
|----|---------------------|---------|
| 13 | NMR of Other Nuclei | Chapt 6 |
|----|---------------------|---------|

Stereochemistry

- | | | |
|-------|--|----------|
| 14-15 | <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 Presentations

16 **FINAL** (Take-home; available 4/28, 8:00 AM; due 5/4, 5:00 PM)

University Policies and Procedures:

COVID-19 Classroom Safety Protocols

While not mandated, USU encourages and welcomes the wearing of masks in all university building, especially within 6 feet of others. Furthermore, it is strongly encouraged to take measures to mitigate risk as recommended by federal and state public health officials. These measures include getting fully vaccinated, staying home if you are sick (even with mild symptoms), and maintaining good hygiene including frequent hand washing. Testing will be provided, without charge, throughout the semester and the [USU COVID Webpage](https://www.usu.edu/covid-19/) [_\(https://www.usu.edu/covid-19/\)_](https://www.usu.edu/covid-19/) will provide up-to-date information. Please

remember; COVID can have significant impact on the health and safety of those around you so remain vigilant and respectful.

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. [USU Policy 403](http://www.usu.edu/hr/files/uploads/Policies/403.pdf) [_\(http://www.usu.edu/hr/files/uploads/Policies/403.pdf\)_](http://www.usu.edu/hr/files/uploads/Policies/403.pdf) further defines academic freedom and professional responsibilities.

Academic Integrity - "The Honor System"

The University expects that students and faculty alike maintain the highest standards of academic honesty. The Code of Policies and Procedures for Students at Utah State University ([Student Conduct](https://studentconduct.usu.edu/studentcode) [_\(https://studentconduct.usu.edu/studentcode\)_](https://studentconduct.usu.edu/studentcode)) addresses academic integrity and honesty and notes the following:

Academic Integrity: Students have a responsibility to promote academic integrity at the University by not participating in or facilitating others' participation in any act of academic dishonesty and by reporting all violations or suspected violations of the Academic Integrity Standard to their instructors.

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". Violations of the Academic Integrity Standard (academic violations) include, but are not limited to cheating, falsification, and plagiarism

Plagiarism

Plagiarism includes knowingly "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. It also includes the unacknowledged use of materials prepared by another person or agency engaged in the selling of term papers or other academic materials." The penalties for plagiarism are severe. They include warning or reprimand, grade adjustment, probation, suspension, expulsion, withholding of transcripts, and denial or revocation of degrees.

Course Fees

Instructors that utilize course fees should identify the amount and explain the purpose of the course fee on the top half of the first page of the syllabus. Course fees are listed in the catalog.

Grievance Process

Students who feel they have been unfairly treated [in matters other than discipline, admission, residency, employment, traffic, and parking - which are addressed by procedures separate and independent from the Student Code] may file a grievance through the channels and procedures described in the Student Code: [Article VII Grievances](https://studentconduct.usu.edu/studentcode/article7) [_\(https://studentconduct.usu.edu/studentcode/article7\)](https://studentconduct.usu.edu/studentcode/article7).

Discrimination and Sexual Misconduct

USU strives to provide an environment for students and employees that is free from [discrimination](https://www.usu.edu/equity/non-discrimination.php) [_\(https://www.usu.edu/equity/non-discrimination.php\)](https://www.usu.edu/equity/non-discrimination.php) and [sexual misconduct](https://www.usu.edu/equity/sexual-misconduct/Sexual-Misconduct-Terms.php) [_\(https://www.usu.edu/equity/sexual-misconduct/Sexual-Misconduct-Terms.php\)](https://www.usu.edu/equity/sexual-misconduct/Sexual-Misconduct-Terms.php). If you experience sexual misconduct or discrimination at any point during the semester inside or outside of class, you are encouraged to contact the [USU Title IX Coordinator](https://www.usu.edu/equity/sexual-misconduct/Title-IX-Coordinator.php) [_\(https://www.usu.edu/equity/sexual-misconduct/Title-IX-Coordinator.php\)](https://www.usu.edu/equity/sexual-misconduct/Title-IX-Coordinator.php) via Old Main room 161 in Logan, [435-797-1266](tel:435-797-1266) [\(tel:1-435-797-1266\)](tel:435-797-1266), titleix@usu.edu [\(mailto:titleix@usu.edu\)](mailto:titleix@usu.edu), or at [equity.usu.edu/report](https://www.usu.edu/equity/report.php) [_\(https://www.usu.edu/equity/report.php\)](https://www.usu.edu/equity/report.php). You can learn more about the USU resources available for individuals who have experienced sexual misconduct at [sexualrespect.usu.edu](https://www.usu.edu/sexual-respect/) [_\(https://www.usu.edu/sexual-respect/\)](https://www.usu.edu/sexual-respect/). Resources for individuals who have experienced discrimination are listed at [equity.usu.edu](https://www.usu.edu/equity/) [_\(https://www.usu.edu/equity/\)](https://www.usu.edu/equity/).

Required Reporting of Sexual Misconduct

The instructor is designated by USU as a "[reporting employee](https://www.usu.edu/equity/sexual-misconduct/employees.php) [_\(https://www.usu.edu/equity/sexual-misconduct/employees.php\)](https://www.usu.edu/equity/sexual-misconduct/employees.php)." This means that if you share information about [sexual misconduct](https://www.usu.edu/equity/sexual-misconduct/Sexual-Misconduct-Terms.php) [_\(https://www.usu.edu/equity/sexual-misconduct/Sexual-Misconduct-Terms.php\)](https://www.usu.edu/equity/sexual-misconduct/Sexual-Misconduct-Terms.php) (sexual harassment, sexual assault, relationship violence, or sex-based stalking) with the instructor, they *will report* that information to the [USU Title IX Coordinator](https://www.usu.edu/equity/sexual-misconduct/Title-IX-Coordinator.php) [_\(https://www.usu.edu/equity/sexual-misconduct/Title-IX-Coordinator.php\)](https://www.usu.edu/equity/sexual-misconduct/Title-IX-Coordinator.php). The instructor is also required to tell you about [designated confidential resources](https://www.usu.edu/sexual-respect/resources.php) [_\(https://www.usu.edu/sexual-respect/resources.php\)](https://www.usu.edu/sexual-respect/resources.php), [supportive measures](https://www.usu.edu/equity/Supportive-Measures.php) [_\(https://www.usu.edu/equity/Supportive-Measures.php\)](https://www.usu.edu/equity/Supportive-Measures.php), and [how you can file a report](https://www.usu.edu/equity/report.php) [_\(https://www.usu.edu/equity/report.php\)](https://www.usu.edu/equity/report.php) with the USU Title IX Coordinator.

Students with Disabilities

USU welcomes students with disabilities. If you have, or suspect you may have, a physical, mental health, or learning disability that may require accommodations in this course, please contact the Disability Resource Center (DRC) as early in the semester as possible (University Inn # 101, 435-797-2444, drc@usu.edu (<mailto:drc@usu.edu>)). All disability related accommodations must be approved by the DRC. Once approved, the DRC will coordinate with faculty to provide accommodations.

Withdrawal Policy, "I" Grade Policy and Dropping Courses

If a student does not attend a class during the first week of the term or by the second class meeting, whichever comes first, the instructor may submit a request to have the student dropped from the course. (This does not remove responsibility from the student to drop courses which they do not plan to attend.) Students who are dropped from courses will be notified by the Registrar's Office through their preferred e-mail account.

Students may drop courses without notation on the permanent record through the first 20 percent of the class. If a student drops a course following the first 20 percent of the class, a W will be permanently affixed to the student's record (check [General Catalog](https://catalog.usu.edu/misc/catalog_list.php?catoid=12) [_\(https://catalog.usu.edu/misc/catalog_list.php?catoid=12\)_](https://catalog.usu.edu/misc/catalog_list.php?catoid=12) for exact dates).

Students with extenuating circumstances should refer to the policy regarding Complete Withdrawal from the University and the Incomplete (I) Grade policy in the General Catalog.

No-Test Days Policy

For classes that meet for a full semester, a five-day period designated as "no-test" days precedes final examinations. During this time, no major examinations, including final examinations will be given in order that students may concentrate on classwork, the completion of special assignments, writing projects, and other preparation for duly scheduled final examinations. Approved exceptions include final papers, weekly chapter quizzes, quizzes, projects, and examinations associated with a lab that does not meet during final examinations. This policy does not apply to classes that meet only during the second 7-week session of the semester or to classes offered during the summer term. Complete information related to [Final Examination Policies](https://catalog.usu.edu/content.php?catoid=12&navoid=3311) [_\(https://catalog.usu.edu/content.php?catoid=12&navoid=3311\)_](https://catalog.usu.edu/content.php?catoid=12&navoid=3311) can be reviewed in the General Catalog.

Assumption of Risk

All classes, programs, and extracurricular activities within the University involve some risk, and some involve travel. The University provides opportunities to participate in these programs on a voluntary basis. Therefore, students should not participate in them if they do not care to assume the risks. Students can ask the respective program leaders/sponsors about the possible risks a program may generate, and if students are not willing to assume the risks, they should not select that program. By






voluntarily participating in classes, programs, and extracurricular activities, students do so at their own risk. General information about University Risk Management policies, insurance coverage, vehicle use policies, and risk management forms can be found at <http://www.usu.edu/riskmgmt/> (<http://www.usu.edu/riskmgmt/>).








Mental Health

Mental health is critically important for the success of USU students. As a student, you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance or reduce your ability to participate in daily activities. Utah State University provides free services for students to assist them with addressing these and other concerns. You can learn more about the broad range of confidential mental health services available on campus at [Counseling and Psychological Services \(CAPS\)](https://counseling.usu.edu/) (<https://counseling.usu.edu/>).

Students are also encouraged to download the [“SafeUT App”](https://healthcare.utah.edu/uni/programs/safe-ut-smartphone-app) (<https://healthcare.utah.edu/uni/programs/safe-ut-smartphone-app>) to their smartphones. The SafeUT application is a 24/7 statewide crisis text and tip service that provides real-time crisis intervention to students through texting and a confidential tip program that can help anyone with emotional crises, bullying, relationship problems, mental health, or suicide related issues.

Course Summary:

Date	Details	Due
Tue Jan 11, 2022	 Pre-Test (https://usu.instructure.com/courses/682442/assignments/3573361)	due by 11:59pm
Wed Jan 12, 2022	 Pre-Test (https://usu.instructure.com/courses/682442/assignments/3573353)	due by 11:59pm
Mon Feb 7, 2022	 Homework 1 (https://usu.instructure.com/courses/682442/assignments/3573352)	due by 11:59pm
Thu Feb 10, 2022	 Homework 2 (https://usu.instructure.com/courses/682442/assignments/3573351)	due by 11:59pm
Mon Feb 21, 2022	 Homework 3 (https://usu.instructure.com/courses/682442/assignments/3573350)	due by 11:59pm

Date	Details	Due
Fri Feb 25, 2022	 CHEM 7310 Exam 1 (https://usu.instructure.com/courses/682442/assignments/3573354)	due by 11:59pm
Thu Mar 10, 2022	 Homework4 (https://usu.instructure.com/courses/682442/assignments/3573357)	due by 11:59pm
Mon Apr 4, 2022	 Homework 5 (https://usu.instructure.com/courses/682442/assignments/3573358)	due by 11:59pm
Thu Apr 7, 2022	 CHEM 7310 Exam 2 (https://usu.instructure.com/courses/682442/assignments/3573355)	due by 11:59pm
Mon Apr 18, 2022	 Homework 6 (https://usu.instructure.com/courses/682442/assignments/3573359)	due by 11:59pm
Fri Apr 22, 2022	 Final Exam (https://usu.instructure.com/courses/682442/assignments/3573356)	due by 11:59pm
	 Presentation (https://usu.instructure.com/courses/682442/assignments/3573360)	