

Course Syllabus

Chemistry 5235/4230 (Section 11526/11596) Organic Spectroscopy Fall 2020

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Lectures: Tuesday Period 4-5 10:40am - 12:35 via ZOOM

Problem sessions: Thursday Period 4: 10:40am - 11:30 via Zoom on 9/17; 10/01; 10/15; 10/29; 11/12; 12/03.

The problem session is required for CHM 5235 students and participation will be graded. CHM 4230 students are highly encouraged to attend the problem session.

Office hours: Thursday Period 4: 10:40 - 11:30 or by appointment via Zoom.

Course texts:

1. **Spectrometric Identification of Organic Compounds (Silverstein, 8th or 7th ed.)**
Or: Introduction to Spectroscopy (Pavia, Lampman, Kriz, Vyvyan, 5th ed.)
Or: Organic Structure Analysis (Crews, Rodriguez, Jaspars, 2nd ed.)
2. **Structure Determination of Organic Compounds: Tables of Spectral Data (E. Pretsch, 4th ed.)**

(NMR theory, grad student level: Basic One- and Two-dimensional NMR Spectroscopy (H. Friebolin, 5th ed.)

Or: Understanding NMR Spectroscopy (J. Keeler, 2nd ed.)

Or: High-Resolution NMR Techniques in Organic Chemistry (T. Claridge))

E-Learning: We will use a Canvas site: <https://lss.at.ufl.edu/> (check regularly to find announcements, lecture notes and handouts, exam scores, and other information related to this class). From this webpage, click on the Canvas login button and then use your Gatorlink ID to log in.

Prerequisites: One year of organic chemistry (CHM 2210/2211) is necessary.

Course description and objectives: Survey of spectroscopic techniques used to elucidate the structures of unknown organic compounds. These topics will include mass spectrometry, infrared and ultraviolet spectroscopy, 1- and 2-dimensional NMR applications. Beside theory and fundamentals of these techniques, the major emphasis is to enable students to elucidate structures of various complexities by illustrated examples, guided in-class exercises, and working on weekly problem sets.

Course learning outcomes

By the end of this course, students will be able to:

1. Distinguish spectroscopic techniques (UV, IR, NMR, MS) and plan hands-on experiments.
2. Use different modern NMR, IR, and mass spectrometry techniques to determine the structure of a complex, unknown organic compound.
3. Understand and be able to optimize modern multi-dimensional NMR techniques such as COSY and 2D heteronuclear experiments.
4. Design their own multi-dimensional NMR experiments for specific purposes.
5. Be able to critically evaluate and discuss techniques used in the literature.

Evaluation	CHM 5235	CHM 4230
Exam 1 (in class)	30%	45%
Exam 2 (in class)	30%	35%
Exam 3 (take home)	20%	25%
Problem Sets (5 sets)	20%	-

Here is a [link to the university grades and grading policies](#). This is a problem-solving class; thus, your grade will be largely determined by how well you interpret the various types of spectral problems. I will introduce each spectroscopic technique with 1-3 lectures including demonstrations and problem sets (5) will follow each paragraph. Problem sets are take-home assignments; the due date will be announced in class. Midterm and Final are in-class exams and will be mostly on determining the connectivity and stereochemistry of organic compounds from spectral data provided. You will be able to use your notes and the textbooks.

It is **critical** that you attend every lecture session or watch the recording/notes timely, as we will be covering significant amounts of material daily and demonstrating problem-solving techniques. There are no make-up quizzes (if an exam/problem set is missed with approved absence, the final grade will replace it. Requirements for class attendance and make-up exams, assignments, and other work in this course are consistent with university policies. [Click here to read the university attendance policies](#).

Classroom Policies

Students are expected to behave in a professional manner at all times. Positive contributions to the learning environment and participation in classroom learning activities are expected. Students should demonstrate courtesy to the instructor, as well as to their fellow classmates. Focusing your attention on anything other than pertinent classroom material could be considered discourteous.

Our class sessions may be audio visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Student Honor Code

The UF Student Honor Code (see <http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/> for details): We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." Honor Code violations include copying on an exam (or helping another student to copy) and/or turning in an exam for regrading that has been changed since it was graded by the instructor.

Any student found responsible for an academic honesty violation in this course will be recommended sanctions consistent with the offense.

Other Important Information

- Disability Resources: Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center. [Click here to get started with the Disability Resource Center](#). It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.
- Division of Student Affairs (Counseling, Dean of Students Office): <http://www.ufsa.ufl.edu/>.
- Need help dropping this class? Contact a Chemistry undergraduate advisor here: <https://www.chem.ufl.edu/undergraduate/advising/>

- Your well-being is important to the University of Florida. The U Matter, We Care initiative (<http://www.umatter.ufl.edu/>) is committed to creating a culture of care on our campus by encouraging members of our community to look out for one another and to reach out for help if a member of our community is in need. If you or a friend is in distress, please contact umatter@ufl.edu so that the U Matter, We Care Team can reach out to the student in distress. A nighttime and weekend crisis counselor is available by phone at 352-392-1575. The U Matter, We Care Team can help connect students to the many other helping resources available including, but not limited to, Victim Advocates, Housing staff, and the Counseling and Wellness Center. Please remember that asking for help is a sign of strength. In case of emergency, call 9-1-1.
- Online course evaluation: Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. [Click here for guidance on how to give feedback in a professional and respectful manner.](#) Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals. [Summaries of course evaluation results are available to students here.](#)

ALL DATES AND ASSIGNMENTS ARE TENTATIVE AND SUBJECT TO CHANGE.

Date	Theme	PS	Topics (textbook chapters)
9/01/20_A	MS 1		Syllabus, Intro MS, CH1
9/01/20_B	MS 2		CH1 [theory, EI, CI ionization]
9/08/20_A	MS 3		CH1 [ESI, MALDI, FAB]
9/08/20_B	MS 4		CH1 [mass detectors, halogens, degree of unsaturation, fragmentation]
9/15/20_A	MS 5	1 out	CH1 [MS summary slides]
9/15/20_B	IR 1		CH2
9/22/20_A	IR 2		CH2
9/22/20_B	UV-Vis	1 back	Extra hand out (not in Silverstein book)
9/29/20_A	NMR 1	2	CH3 [theory: nuclear spin, resonance, NMR spectrometer, magnetization, relaxation]
9/29/20_B	NMR 2		CH3 [chemical shift, Integration, coupling, coupling constant J]
10/06/20_A	NMR 3	2	CH3 [chemical and magnetic equivalence, examples]
10/06/20_B	NMR 4		CH3 [first order, higher order spectra, Pople notation, multiplets]
10/13/20_A	NMR 5		CH3 [multiplets analysis, Hoyer, second order spectra, exercises]
10/13/20_B	NMR 6		CH3 [calculating shifts, solvents, data reporting, dynamic NMR]
10/20/20_A	NMR 7	3	CH3 [line width, coalescence, Eyring equation, proton exchange]
10/20/20_B	NMR 8		CH4 [C 13 NMR, theory, decoupling, chemical shift range, DEPT]
10/27/20	Exam 1 10:40am -12 real time, online		
11/03/20	NMR 9	3	Catch up, example for 1mg vs 10 mg, 400 vs 700 MH

11/03/20	NMR 2D 1		CH5 [Intro 2D NMR, COSY, TOCSY, 2D COSY, selective TOCSY]
11/10/20_A	NMR 2D 2		CH5 [Types of C-H exp, HMQC, HMBC, inadequate]
11/10/20_B	NMR 2D 3		CH5 [NOE, difference NOE, 2D NOESY]
11/17/20_A	NMR 2D 4	4	CH5 [through space correlations, examples, NMR history]
11/17/20_B	NMR 2D 5		CH5 [2D training with Ipsenol, 8.27 & 8.32 Silverstein]
11/24/20_A	Stereochemistry 1	4	Stereochemistry start, acetamide
11/24/20_B	Stereochemistry 2		Stereochemistry: Kishi's database, Mosher's Ester
12/01/20_A	Stereochemistry 3	5	Stereochemistry: Murata's J-based, NMR calculations, Marfey's analysis, optical rotation, ECD, hexacyclinol story
12/01/20_B	Stereo/Other Nuclei		CH6 [15N, protein NMR, STD NMR, examples]
12/08/20_A	Other Nuclei	5	CH6 [2H, 19F, 29Si, 31P, 119Sn, examples]
12/08/20_B	Exam prep		Catch up topics, practice old final, Questions??
12/17/2020	<i>Exam 2: 2h real time, online 7:30-9:30am,</i>		
12/16-12/18	<i>Exam 3: 48h take-home assignment (online 12/16 2pm, due 12/18 2pm)</i>		