

# Chemistry 4361/8361: Interpretation of Organic Spectra

## *Syllabus and Course Information*

- Course Description:** CHEM 4361/8361 is an introduction to practical analysis of organic compounds using spectrometric and spectroscopic tools. In this course, we will cover applications of nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry (MS), and ultraviolet-visible (UV) and infrared (IR) spectroscopy. The class offers students tools to determine structures in a research environment, with an emphasis on practice. For CHEM 8361, there is a lab component (MS and NMR).
- Instructor:** Phil Buhlmann, 325 Smith Hall, office 612-624-1431  
E-Mail: [buhlmann@umn.edu](mailto:buhlmann@umn.edu)
- Teaching Assistant:** Vilma Brandao, 14/18 Smith Hall, 612-625-9093  
E-mail: [bran1222@umn.edu](mailto:bran1222@umn.edu)
- Lectures:** Mo, W, F, 9:05 to 9:55 AM; Room 110 Tate Hall  
Laboratory time to be announced
- Active participation in this course is expected and helps you and your fellow class members. This is best achieved by attendance of class in person, the default participation mode. However, lectures will be recorded by Zoom and made available to those registered for this course as well as class guests. This will benefit those who miss a class because of an excused absence, or simply because they think they benefit from reviewing the class. *Sharing of class recordings and other materials used in this class (other than your own class notes) with individuals outside of this class is a violation of the student conduct code.* Please let me know if you have any concerns.
- COVID:** Per current university policies, masks must be worn in the classroom. Students not complying will be asked to leave the classroom.
- For your own protection, please leave every 2<sup>nd</sup> seat unoccupied, and use the same seat throughout the semester.
- I will do my very best to accommodate your needs. If you don't feel well or think you have been exposed to COVID, we all prefer that you do not come to class and consult the Boynton Nurse Line at **612-625-3222**, <https://provost.umn.edu/covid-19-response/guidance-student-positive-cases>.
- Office Hours:** Instructor office hours specific to this class and as mental health advocate: Per appointment; format: typically Zoom.
- Combined in-person office hours for this class and as mental health advocate: Monday, noon to 1:00 PM, Smith 325. Privacy per your needs.
- Web Page:** Canvas (<https://canvas.umn.edu/courses/267784>)
- Required Text:** E. Pretsch, P. Bühlmann & C. Affolter, *Structure Determination of Organic Compounds* (5<sup>th</sup> ed.; Springer, Berlin, 2020). Available at the University of Minnesota library at the following site:
- <https://link-springer-com.ezp3.lib.umn.edu/book/10.1007%2F978-3-662-62439-5>

*Other books that you may find useful:*

J. B. Lambert, S. Gronert, H. F. Shurvell, & D. A. Lightner, *Organic Structural Spectroscopy* (2<sup>nd</sup> ed.; Pearson-Prentice Hall, Upper Saddle River, NJ, 2011).

T. Claridge, *High-Resolution of NMR Techniques in Organic Chemistry* (Elsevier, 2016).

J. Keeler, *Understanding NMR Spectroscopy* (2<sup>nd</sup> ed.; Wiley, 2010). Notes from the authors available on line: <http://www-keeler.ch.cam.ac.uk/lectures/>

P. Crews, J. Rodriguez, M. Jaspars, *Organic Structure Analysis* (Oxford University Press, New York, 1998).

J. B. Lambert, H. F. Shurvell, D. A. Lightner, R. G. Cooks, *Organic Structural Spectroscopy* (Prentice-Hall, Upper Saddle River, NJ, 1998).

E. Breitmaier, *Structure Elucidation by NMR in Organic Chemistry: A Practical Guide* (Wiley, New York, 2002)

T. D. W. Claridge, *High-Resolution NMR Techniques in Organic Chemistry* (Second Edition) (Elsevier, Oxford, 2009)

S. Berger, S. Braun, *200 and More NMR Experiments* (Wiley, New York, 2004)

J. C. Hollerton, S. A. Richards, *Essential Practical NMR for Organic Chemistry* (Wiley, West Sussex, UK, 2011)

E. de Hoffmann, V. Stroobant, *Mass Spectrometry: Principles and Applications* (Wiley, New York, 1999)

F. W. McLafferty, F. Turecek, *Interpretation of Mass Spectra* (University Science Books (Mill Valley, CA, 1993).

D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, *Introduction to Spectroscopy* (Cengage Learning, Stamford, CT, 2015)

**Quizzes:**

Quizzes are administrated **every Friday (except for the first week of classes and a few other exceptions; see schedule)**. Quizzes are 10–15 min long and include questions regarding the entire course. Quizzes are open-book and students are allowed to use their own notes but may not get any help from other individuals.

**Exams:**

There will be two exams during the semester. The final exam will be comprehensive. Exams are open-book and students are allowed to use their own notes but may not get any help from other individuals.

Grading CHEM4361 (3 credits): 60% midterms, 30% final, 10% quizzes.

Grading CHEM8361 (4 credits): 55% midterms, 25% final, 10% quizzes, 10% lab.

**Laboratory:**

Labs will be conducted *in person* in the Chemistry Department NMR Facility and Mass Spectrometry Facility. Labs are required for all students enrolled in Chem 8361. Instructions for writing up each lab are in the lab instructions. Lab times will be organized by the course TA; expect about 2 to 3 hours for the MS and NMR lab each, plus lab report preparation.

**Any Type of Feedback:** Always **very** welcome. If you want to keep your comments anonymous, put them into mailbox C2 in front of room 139 Smith Hall.

**Regrading Exams:** Regrades can and will be honored, provided that the following conditions are met:

1. The request for the regrade, along with the specific reasons for your request, are presented in writing along with your exam.
2. The request is made within five working days of the day the graded exam was returned to the student.
4. The entire exam will be subject to a regrade.

## ***Policies That Apply to All My Courses That Are Equally Important***

### ***Makeup Work for Legitimate Absences***

***Missed Exams:*** In the case of a true emergency, serious illness, or University-related trip that prevents a student from taking a midterm exam, an excused absence may be granted in strict accordance with University policy (see link below). To obtain an excused absence, students must contact the instructor in advance OR as soon as circumstances allow to discuss the nature of the emergency. Documentation will be required. If circumstances prevent a student from taking more than one quizzes or exams, the student must contact the instructor as soon as possible to schedule a meeting to discuss options available. <http://www.policy.umn.edu/Policies/Education/Education/MAKEUPWORK.html>

Students on University teams playing out of town may be able to take the exam with the coach or an instructor as proctor; please see the course instructor about this early so arrangements can be made. For information on missing the final exam, see "Incompletes".

***Incompletes:*** Students who have an EXCUSED ABSENCE from the Final Exam, and have taken the midterm exam, may be eligible to receive a grade of "I" in the course. Incompletes will not be granted if a student has missed midterm exams, or is not passing based on the work up to the final. You need to fill out an incomplete request form (available in Smith 115) and have it signed. See me for details. This grade is NOT routinely assigned! Any incomplete must be made up in the following semester. After that time all incompletes will turn into F grades.

### ***Student Conduct Code***

The University seeks an environment that promotes academic achievement and integrity, that is protective of free inquiry, and that serves the educational mission of the University. Similarly, the University seeks a community that is free from violence, threats, and intimidation; that is respectful of the rights, opportunities, and welfare of students, faculty, staff, and guests of the University; and that does not threaten the physical or mental health or safety of members of the University community.

As a student at the University you are expected adhere to Board of Regents Policy: *Student Conduct Code*. To review the Student Conduct Code, please see: [http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student\\_Conduct\\_Code.pdf](http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf).

Note that the conduct code specifically addresses disruptive classroom conduct, which means "engaging in behavior that substantially or repeatedly interrupts either the instructor's ability to teach or student learning. The classroom extends to any setting where a student is engaged in work toward academic credit or satisfaction of program-based requirements or related activities."

### ***Use of Personal Electronic Devices in the Classroom***

Using personal electronic devices in the classroom setting can hinder instruction and learning, not only for the student using the device but also for other students in the class. To this end, the University establishes the right of each faculty member to determine if and how personal electronic devices are allowed to be used in the classroom. For complete information, please reference: <http://policy.umn.edu/education/studentresp>.

### ***Scholastic Dishonesty***

You are expected to do your own academic work and cite sources as necessary. Failing to do so is scholastic dishonesty. Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis. (Student Conduct Code: [http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student\\_Conduct\\_Code.pdf](http://regents.umn.edu/sites/regents.umn.edu/files/policies/Student_Conduct_Code.pdf)) If it is determined that a student has cheated, the student may be given an "F" or an "N" for the course, and may face additional sanctions from the University. For additional information, please see: <http://policy.umn.edu/education/instructorresp>.

The Office for Community Standards has compiled a useful list of Frequently Asked Questions pertaining to scholastic dishonesty: <https://communitystandards.umn.edu/avoid-violations/avoiding-scholastic-...>. If you have additional questions, please clarify with your instructor for the course. Your instructor can respond to your specific questions regarding what would constitute scholastic dishonesty in the context of a particular class-e.g., whether collaboration on assignments is permitted, requirements and methods for citing sources, if electronic aids are permitted or prohibited during an exam.

### ***Appropriate Student Use of Class Notes and Course Materials***

Taking notes is a means of recording information but more importantly of personally absorbing and integrating the educational experience. However, broadly disseminating class notes beyond the classroom community or accepting compensation for taking and distributing classroom notes undermines instructor interests in their intellectual work product while not substantially furthering instructor and student interests in effective learning. Such actions violate shared norms and standards of the academic community. For additional information, please see: <http://policy.umn.edu/education/studentresp>.

### ***Sexual Harassment***

"Sexual harassment" means unwelcome sexual advances, requests for sexual favors, and/or other verbal or physical conduct of a sexual nature. Such conduct has the purpose or effect of unreasonably interfering with an individual's work or academic performance or creating an intimidating, hostile, or offensive working or academic environment in any University activity or program. Such behavior is not acceptable in the University setting. For additional information, please consult Board of Regents Policy: [https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual\\_Harassment\\_Sexual\\_Assault\\_Stalking\\_Relationship\\_Violence.pdf](https://regents.umn.edu/sites/regents.umn.edu/files/policies/Sexual_Harassment_Sexual_Assault_Stalking_Relationship_Violence.pdf)

The Aurora Center provides an additional source of support and help: <http://aurora.umn.edu>

### ***Equity, Diversity, Equal Opportunity, and Affirmative Action***

The University provides equal access to and opportunity in its programs and facilities, without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression. For more information, please consult Board of Regents Policy: [http://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity\\_Diversity\\_EO\\_AA.pdf](http://regents.umn.edu/sites/regents.umn.edu/files/policies/Equity_Diversity_EO_AA.pdf).

For the Gender and Sexuality Center for Queer and Trans Life, see: <https://gsc.umn.edu/>

For gender-neutral restrooms in Smith and Kolthoff Halls and elsewhere on campus, see: <https://sites.google.com/umn.edu/chemintranet/accessible-gender-neutral-restrooms>

### ***Disability Accommodations***

The University of Minnesota views disability as an important aspect of diversity, and is committed to providing equitable access to learning opportunities for all students. The Disability Resource Center (DRC) is the campus office that collaborates with students who have disabilities to provide and/or arrange reasonable accommodations.

- If you have, or think you have, a disability in any area such as, mental health, attention, learning, chronic health, sensory, or physical, please contact the DRC office on your campus (UM Twin Cities - [612.626.1333](tel:612.626.1333)) to arrange a confidential discussion regarding equitable access and reasonable accommodations.
- Students with short-term disabilities, such as a broken arm, **can** often work with instructors to **minimize** classroom barriers. In situations where additional assistance is needed, students should contact the DRC as noted above.
- If you are registered with the DRC and have a disability accommodation letter dated for this semester or this year, please contact your instructor early in the semester to review how the accommodations will be applied in the course.
- If you are registered with the DRC and have questions or concerns about your accommodations, please contact your (access consultant/disability specialist). Additional information is available on the DRC website: <https://diversity.umn.edu/disability/home> ([drc@umn.edu](mailto:drc@umn.edu)).
- For accessible restrooms in Smith and Kolthoff Halls, see <https://sites.google.com/umn.edu/chemintranet/accessible-gender-neutral-restrooms>

### ***Mental Health and Stress Management***

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 and may reduce your ability to participate in daily activities. University of Minnesota services are available to assist you. You can learn more about the broad range of confidential mental health services available on campus via the Student Mental Health Website: <http://www.mentalhealth.umn.edu>.

### ***Academic Freedom and Responsibility: for courses that do not involve students in research***

Academic freedom is a cornerstone of the University. Within the scope and content of the course as defined by the instructor, it includes the freedom to discuss relevant matters in the classroom. Along with this freedom comes responsibility. Students are encouraged to develop the capacity for critical judgment and to engage in a sustained and independent search for truth. Students are free to take reasoned exception to the views offered in any course of study and to reserve judgment about matters of opinion, but they are responsible for learning the content of any course of study for which they are enrolled. Reports of concerns about academic freedom are taken seriously, and there are individuals and offices available for help. Contact the instructor, the Department Chair, your adviser, the associate dean of the college, or the Vice Provost for Faculty and Academic Affairs in the Office of the Provost.

## Approximate Lecture and Exam Schedule

	Topic	Annotations
Wed 9/8	Introduction to the course & MS Introduction	
Fri 9/10	MS: Molecular Formula: Determination and Index of hydrogen deficiency	
Mon 9/13	MS: Molecular Formula: Determination and Index of hydrogen deficiency	
Wed 9/15	MS: Fragmentation and MS of some chemical classes	
Fri 9/17	MS: Problem solving	Quiz #1
Mon 9/20	MS: Fragmentation and MS of some chemical classes	
Wed 9/22	Fragmentation in ESI MS	
Fri 9/24	MS: Problem Solving	Quiz#2
Mon 9/27	Infrared Spectroscopy (IR): principles and applications	
Wed 9/29	IR: Characteristic group absorptions of organic molecules	
Fri 10/1	MS, IR: Problem Solving	Quiz#3
Mon 10/4	IR: Characteristic group absorptions of organic molecules	
Wed 10/6	Nuclear Magnetic Resonance (NMR):Introduction	
Fri 10/8	MS, IR, NMR: Problem Solving	Quiz#4
Mon 10/11	<sup>1</sup> H NMR Spectroscopy: Spin-spin coupling	
Wed 10/13	<sup>1</sup> H NMR Spectroscopy: Exchange phenomena	
Fri 10/15	Midterm I	No Quiz
Mon 10/18	NMR Spectroscopy: Relaxation, Longitudinal and transverse relaxation times	
Wed 10/20	NMR: Detecting and processing NMR signals	
Fri 10/22	NMR: Problem Solving	Quiz#5
Mon 10/25	NMR: 1D and 2D homonuclear spectra	
Wed 10/27	NMR: 1D and 2D homonuclear spectra	
Fri 10/29	NMR: Problem Solving	Quiz#6
Mon 11/1	NMR: COSY, ROESY, and NOESY experiments	
Wed 11/3	NMR: COSY, ROESY, and NOESY experiments	
Fri 11/5	Mass Spectrometry: Instrumentation [Joe Dalluge]	
Mon 11/8	NMR: HSQC and HMBC experiments	
Wed 11/10	NMR: 2D INADEQUATE experiment	
Fri 11/12	NMR: Problem Solving	Quiz#7
Mon 11/15	NMR: Heteronuclear NMR	
Wed 11/17	Nuclear Magnetic Resonance (NMR): Doing it in the lab [Letitia Yao]	
Fri 11/19	NMR: Problem Solving	No Quiz
Mon 11/22	MIDTERM#2	
Wed 11/24	NMR: Determining stereochemistry	
Fri 11/26	THANKSGIVING!	
Mon 11/29	NMR: Advanced NMR techniques	
Wed 12/1	NMR: Advanced NMR techniques	
Fri 12/3	Problem solving	Quiz#8
Mon 12/6	Ultraviolet-visible (UV) spectroscopy: Principles and applications	
Wed 12/8	Ultraviolet-visible (UV) spectroscopy: Principles and applications	
Fri 12/10	Problem solving	Quiz#9
Mon 12/13	Putting it all together	
Wed 12/15	Problem solving	
Mon 12/20	FINAL EXAM (1:30 to 3:30 PM)	