

CHEMISTRY 442

Spectroscopy and Molecular Structure

Fall 2009 Syllabus

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Course Schedule:

Lecture:	MWF 11:30 – 12:20	Room 215
Lab Sections:	Th 7:45 - 11:35 am	Room 239

Office Hours: By appointment or walk-in.

Course Description: We will examine the modern techniques for the structural elucidation of organic molecules, including IR, NMR and mass spectrometry. Both theory and applications will be addressed with an emphasis on problem solving.

Course Objectives: The overall objective is to become proficient at using MS, IR, and NMR for organic structure determination. To this end, you should be able to:

- Understand the theory behind mass spectroscopy, infrared spectrometry and nuclear magnetic resonance spectroscopy.
- Have a working knowledge of how these instruments function.
- Be able to interpret the spectra generated by each technique.
- Be able to identify which technique will be the most useful in obtaining an answer to a specific structural question.
- Use data from multiple techniques to arrive at a structure.

Text and Materials:

• "Spectrometric Identification of Organic Compounds" 7th edition, Silverstein, Webster and Kiemle, 2005.

Please bring your book to class!

- Bound laboratory notebook (Freeman).
- Your old 220-221 lab manual.
- Safety glasses or goggles.
- Calculator – Please note that the Chemistry Department does not permit the use of programmable calculators or web-enabled devices during exams or quizzes.
- Moodle site. The "enrollment key" is chem446 (all lower case, no spaces).

Grading Criteria:	Homework	60 pts
	Quizzes	75 pts
	Exams	300 pts
	Laboratory	130 pts
	Participation	10 pts
	<u>Final (cumulative)</u>	<u>125 pts</u>
	Total	700 pts

Letter grades will be assigned as follows: A (630-700), B (560-630), C (490-560), D (420-490), F (420 or below). Keep in mind that +/- grades are included in the ranges shown above. Please be aware that you must earn a passing grade in both the lecture and laboratory to pass the course.

Homework will be assigned on a near-daily basis and some assignments will be collected at the beginning of class. Late homework will not be accepted. Grades will be assigned based on completion and overall quality. Be sure to show all work: present your answers as if you are trying to convince me that your structural assignment is correct. Answers that provide a structure with no explanation will receive little credit. Answer keys will be posted on Moodle.

Exams and Quizzes: There will be 3 quizzes and 3 midterm exams. Quizzes are intended to encourage you to stay current with the work and to help you identify "trouble spots" before taking the exams. The exams will be administered in lab on **October 1, November 5, and December 3**. The final exam is scheduled for **Wednesday, December 16 at 8:30 am**. Tentative quiz dates are listed on the course outline.

Lab: The lab grade consists of the total of three lab reports (40 points each) and a grade on lab technique and etiquette (10 points). Lab technique and etiquette include: preparedness for lab, punctuality, proper handling of chemicals *and instruments*, lab hygiene, and group etiquette. Careful planning and preparation before you arrive at the lab will allow you to complete your experiments in an efficient and safe manner. Missing or arriving late to prelab will result in a reduced grade and may also result in dismissal from the lab. Unsafe behavior in the lab will not be tolerated and repeated violations during a class may result in a zero for that lab. Lab safety and policy will be addressed at the first lab meeting. The lab syllabus is on the last page of this handout.

Attendance is expected and I will take attendance at each class meeting. Attendance at exams, quizzes and labs is mandatory and make-ups are not permitted EXCEPT in cases where: (1) I have been notified of the absence beforehand, and (2) the absence is for a purpose I deem legitimate (major illness, family emergency). The final exam grade (%) will be substituted for an exam that is missed due to an excused absence. Should we have an outbreak of Swine Flu, more liberal attendance policies will take effect. If you have flu symptoms, the College recommends that you not attend class until your symptoms have abated. If you need to miss a quiz, exam or lab due to the flu, please notify me by e-mail **as soon as possible**.

Participation: I like to run this course as a workshop and expect everyone to make a contribution to the discussion. A portion of the grade is based on participation – each time you contribute to the discussion in a meaningful way, you earn a point (up to 10 points). Come to class ready to work spectra and to teach your fellow students your strategies for solving spectra. The key to success in this course is to work as many spectral problems as possible – in and out of class.

Academic Dishonesty, such as copying the work of another or allowing someone else to copy your work and submit it as his/her own, whether it is on an exam, quiz, lab report or homework assignment, will not be tolerated. Penalties for academic dishonesty range from receiving a failing grade on the assignment to dismissal from the college, depending on the nature of the offense. For more information regarding the College policy on academic dishonesty, consult the *Student Handbook*.

Cell Phones: Cellular phones are not permitted in class or in the lab. Please turn off your phone before class or lab and keep it in your backpack or purse.

Extra Credit: Extra credit points (2) can be earned by attending departmental colloquia, up to a maximum of 12 points. If you are unable to attend colloquia due to a conflict with class or practice, you may opt to write summaries of relevant journal articles (see me for details).

Course Outline (Subject to Change)

Every effort will be made to stick to the schedule outlined on the next two pages. Keep in mind that it is quite possible that we may get ahead or behind the schedule by a day or two, or that we may choose to spend additional time on a topic due to class interest. If you have any questions regarding the schedule, please ask!

A few notes regarding the schedule:

- All exams will be given on Thursdays, during the lab period. These dates will not be changed, barring some unforeseen and unusual situation!
- Quiz dates are tentative and may vary depending on our progress with the lecture material. If we need to move a quiz, I will make every effort to give at least a week's notice.
- Reading assignments are given on the syllabus. Read the assignments before class. Homework assignments will be given throughout the semester. You should begin working on the homework assignment as soon as possible (after we cover the material in class). Although the assignments may consist of only a few problems, please realize that some spectral problems may require a considerable amount of analysis (and time).
- I have found that even simple spectral problems can become incredibly difficult if I have not had enough sleep or can not concentrate well for some reason....so plan ahead!

One final thought...

Every chemist develops his or her own method for solving problems. This is especially true in spectroscopy. The only way anyone ever becomes proficient at solving spectral problems is by working lots of problems, making mistakes and learning from those mistakes. Try not to get frustrated if the problems seem tough at first--with patience and practice they get a lot easier. And remember, I am always willing to work with you and answer your questions. Most importantly, have fun!! What other class gives you credit for working puzzles?!?!

Course Schedule:

Date	Topic	Reading
Week 1		
8/31	Introduction, degree of unsaturation	
9/2	Elemental analysis, introduction to MS	1.1-2
9/4	MS instrumentation	1.3-4
Week 2		
9/7	Determination of MW and formula	1.5
9/9	Major fragmentation pathways	1.5-6
9/11	Structural information from fragmentation	1.6
Week 3		
9/14	Fragmentation	1.6
9/16	Practice problems	
9/18	IR theory	2.1-2
Week 4		
9/21	IR instrumentation and practical considerations	2.3-4
9/23	Interpretation of spectra, functional group absorptions	2.5
9/25	Functional group absorptions	2.6
Week 5		
9/28	Functional group absorptions	2.6
9/30	Practice problems	
10/2	NMR review and practice	221 lab manual
Week 6		
10/5	NMR theory	3.1-2
10/7	NMR theory, instrumentation and practical considerations	3.3
10/9	Factors that influence chemical shift	3.4
Week 7		
10/12	Chemical shift	3.4
10/14	Spin-spin coupling	3.5
10/16	Survey of functional groups	
Week 8		

10/19	Heteroatoms	3.6-7
10/21	Karplus, long range coupling	3.13-14
10/23	Tree diagrams, measuring J	3.5
Week 9		
10/26	Practice problems	
10/28	Chemical and magnetic equivalence, chirality	3.8, 9, 12
10/30	Long Weekend, no classes.	
Week 10		
11/2	Popple notation, non-first order coupling, decoupling	3.5, 10, 11
11/4	Practice problems	
11/6	¹³ C NMR: comparison to ¹ H, practical considerations	4.1-2
Week 11		
11/9	C-H coupling, chemical shift	4.3-5
11/11	Chemical shift	4.7
11/13	Chemical shift calculations	4.7
Week 12		
11/16	Practice problems	
11/18	DEPT	4.6
11/20	COSY	5.1-4
Week 13		
11/23	Practice problems	
Week 14		
12/1	HMQC	5.4-5
12/3	Practice problems	
12/5	INADEQUATE	5.6
Week 15		
12/8	Practice problems	
12/10	NOESY, ROESY	5.9
12/12	Practice problems	
Finals	Final Exam is on Wednesday, December 16 at 8:30 am.	

Lab Schedule:

Date:	Experiment:	Techniques:	Due Dates:	Points:
9/3	Check-in and Unknown Structure Determination	CIMS, EIMS, IR, ¹ H NMR		
9/10	Unknown Structure Determination			
9/17	Unknown Structure Determination			
9/24	Reactions of alcohols with Ca(OCl) ₂	MS, IR, ¹ H NMR, ¹³ C NMR		
10/1	Exam 1			
10/8	Reactions of alcohols with Ca(OCl) ₂		Unknown Report Due	40
10/15	Reactions of alcohols with Ca(OCl) ₂			
10/22	Individual Experiments	MS, IR, ¹ H NMR, COSY, DEPT		
10/29	Individual Experiments		Ca(OCl) ₂ Lab Due	40
11/5	Exam 2			
11/12	Individual Experiments			
11/19	Individual Experiments			
11/26	Thanksgiving			
12/3	Exam 3			
12/10	Check-out		Individual Expts. Due	40