

ORGANIC SPECTROSCOPY

Chemistry 572-Fall 2007

Dr. William Jenks

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Lectures:
Tues., Thurs. 2:10 – 3:00 pm 0312 Gilman
Saturday nominally 10:00 am – 12:00 0312 Gilman

Texts: Pretsch, et al., *Structure Determination of Organic Compounds*. 3rd edition.
Crews, et al., *Organic Structure Analysis*
572 Problem Set, from UBS (you will need a 3-ring binder, too)

Office hours: Thursday noon-2:00 p.m or by appointment.
Please come and see me any time or drop me note to arrange a mutually convenient time.

Saturdays:

I'm not much more thrilled about Saturday classes than you are, but as the semester wears on you will see why it works out pretty well. We need to schedule 12 hours of "Saturday morning" lecture at the beginning of the semester, but I need to ask you to be flexible with me. Below is a suggested schedule for the 12 hours:

Sat, Aug 25, 10:30 a.m. – 12:30 p.m.	Thu, Sept 6, 8:00 p.m. – 9:30 p.m.	Thu, Sept 20, 8:00 p.m. – 9:30 p.m.
Thu, Aug 30, 8:00 p.m. – 9:30 p.m.	Thu, Sept 13, 8:00 p.m. – 9:30 p.m.	Sat, Sept 29 10:30 a.m. – 12:30 p.m.

Beginning October 6, we will have a series of 10 exams. The first 9 are on Saturday mornings, and the last is during the final exam period. (Or we could start them a week early and skip the final.) I have traditionally allowed 3 hours for the exams; usually Sat 9 a.m. to noon works best. The exam that should be the weekend before Thanksgiving is done as a take-home.

Grading:

There will be 10 exams and 5 graded homeworks. The exams are traditionally 3 problems each, most of which are structure identifications, with a few essay questions tossed in to keep everyone honest. They can be literally "essays" or other kinds of freeform problems. Each problem on the quizzes will be graded on a scale of 0, 0.5, or 1 point, so the maximum on any given quiz is 3. The graded homeworks will similarly be worth 0, 0.5 or 1. The maximum score in the class is thus 35 points. This class is graded on a sliding scale, meaning that everyone can get an A, though this has yet to happen. By tradition, you need to get 20 points for a B, 25 for an A-, and 27.5 for an A, though I reserve the right to move the scale up or down somewhat to adjust for quizzes that turn out to be harder or easier than I intend. All quizzes are to be done individually. However, they are open-book, open-note with a few restrictions we will discuss in detail later.

Most weeks when there is not a graded homework assignment, there will be an ungraded one. After a while, it will just be my guiding you on where you should be in the problem set book. You are encouraged to work in groups for homeworks and in problem sessions. Solutions will be posted on the web site. It is *imperative* that you do the problems.

Goals and philosophy:

The most obvious goal of this class is for you to learn the skills of interpretation of spectra of organic molecules. You will be able to draw a molecular structure from nothing but spectra. Another important goal, however, is for you to understand how the measurements work so that you can be an intelligent and skilled user. This is critically important from the simple and practical perspective of understanding your spectra and trying to get better data. A large fraction of the lecture time will thus be spent on principles. Interpretation problems will dominate the exams, though, since this is a skill that requires practice and is closely related to your day-to-day activities in the lab. We will go over the exams in class.

Optional problem session

We will arrange a weekly problem session starting about the third week. Attendance is optional, but recommended. A lot of the subtleties of spectral problem solving only come about from practice and seeing the fine points in person.

Final exam:

Thursday December 13, 7:30 a.m. – 11:30 a.m. It's just quiz 10.

Americans with Disabilities Act Compliance. If you have a documented disability and anticipate needing accommodations in this course, please make arrangements with me as soon as possible. Please request that a Disability Resources staff member prepare a SAAR form verifying your disability and specifying the necessary accommodations. Disability Resources is located on the main floor of the Student Services Building in room 1076. Their phone number is 4-7220.

Lecture Topics

The lecture outline below gives an **approximate** outline for 35 "hours" of lecture. Substantial lecture time will also be used to go over exam problems, which will account for the rest of the time of about 40 "hours".

Mass spectrometry	5
principles and instrumentation, fragmentation patterns of functional groups, practical aspects	
Infrared Spectroscopy	5
principles and instrumentation, functional group absorbances, practical aspects, Raman	
Nuclear Magnetic Resonance (NMR) Spectroscopy	
fundamental concepts and vector model	5
solution phase ^1H -NMR	4
solution phase ^{13}C -NMR	2
solid phase ^{13}C -NMR	1
kinetics by NMR, fast and slow timescales	1
2-D experiments and other spin gymnastics	3
Chemically Induced Dynamic Nuclear Polarization (CIDNP)	1
Electron Paramagnetic Resonance (EPR) Spectroscopy	
fundamental concepts, g-factors, coupling, examples,	2
Chemically induced dynamic electron polarization (CIDEP)	1
UV/Visible Spectroscopy	2
Other optical spectroscopies:	
CD and ORD, Fluorescence and Phosphorescence	2