

**Chemistry 3123**  
**Organic Spectral Analysis**  
**Fall 2006**

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Office Hours: M 11pm, Th 9am, and by appointment  
Lectures: T, Th 10:00 – 11:15 AM  
Location: OH 204

***Required:***

**Textbook:** *Introduction to Spectroscopy*, D.L.Pavia, G.M.Lampman, G.S.Kriz, 3<sup>th</sup> Ed., Brooks/Cole, 1998 (ISBN: 0-03-031961-7)

Chemistry 2120 is a prerequisite for this course

***Objectives:***

This class offers an introduction to Organic Structure Analysis. The theory and practical use of modern spectroscopic methods (Ultraviolet/Visible Spectroscopy, CD/ORD Spectroscopy, Infrared Spectroscopy, Mass Spectrometry, and NMR Spectroscopy) will be discussed. The focus of this course is on learning how to approach and systematically deal with spectroscopic problems. A basic discussion of the underlying theory will be offered; however, the application of what you learned to solve current problems (synthesis, natural products, forensics, etc.) will be more important.

***Lectures:***

For most chapters, I will provide lectures notes in advance by email (or webpage), that you should print out and bring to class. These materials will be incomplete (i.e. will have gaps). The idea is that routine information will be written for you and that you will fill in the important information. Thus you can spend more time listening. You will not need these notes, you can just take notes on your own if you prefer.

***Attendance:***

You are strongly encouraged to attend classes. We will solve a lot of example problems in addition to covering the theoretical background to each method. Please be prepared to solve example problems or questions of the problem sets on the board or in smaller groups.

Note: Students with learning disabilities or other disabilities are encouraged to contact me after class to discuss individual needs for accommodations.

***Examinations, Quizzes, and Grading:***

Your progress in this course will be monitored by means of problem sets, midterm examinations and in-class quizzes. There will be four (4) problem sets. I will announce upcoming problem sets in class and either email it or post it on the web. We will have a flexible schedule for these problem sets. Supplying me with just an answer on the problem sets, exams and quizzes is unacceptable. I expect you to write out in a systematic and analytical manner the way you approached the problem and how you arrived at your conclusions. The correct answer is only part of the available credit. The problem sets are due one week after they were handed out.

There are no dates set for the problem sets yet. I will announce them in class and email you the questions. Be prepared to have at least two problem sets in the NMR-part of the lecture!!!

The midterm exams (Wednesday, October 19, and Tuesday, November 22) are necessarily cumulative. You should be prepared to answer questions on both theory and applications (spectroscopic identification). Because of the need for many tables, you may use your book for the exam; however, I reserve the right to remove your book on the exam day if you have written in it extensively. Also, other documentation (notes, tables, etc.) is not allowed. I expect you to answer the problems in the same manner as you answer the problem sets. The Final Exam will cover all material and will most likely consist only of spectra solving problems. Calculators and molecular models are allowed during the exams, however, note that making a model is noisy and uses valuable time.

*Make-up Exams:* The only excuse for missing an exam is illness, authenticated by a physician's statement or a school-related absence. If you miss one exam due to illness or a school-related absence, you will have to take a make-up exam at a later date. If you know that you will be unable to attend one of the exams, you are required to notify me *prior* to the exam so appropriate arrangements can be made. E-mail requests for make-ups immediately prior to or after an exam will not be allowed. This policy will be strictly applied.

The quizzes will be unannounced in-class quizzes. You are expected to solve these spectra problems in a similar way as the exam and problem set problems. The lowest three quiz grades will be dropped.

The course grade will depend on performance on two exams, the five problem sets, the quizzes and the final exam. This course is not graded on a curve. The distribution of course points and the grade cut-offs are as follows:

Midterm examinations (2 x 170)	: 340 pts.
Problem Sets (4 x 80)	: 320 pts.
In-class quizzes	: 100 pts.
<u>Final Examination (1 x 240)</u>	<u>: 240 pts.</u>
<b>Total:</b>	<b>1000 pts.</b>

A	895 -1000	A	935 – 1000
		A-	895 – 934
B	795 – 894	B+	855 – 894
		B	825 – 854
		B-	795 – 824
C	695 – 794	C+	755 – 794
		C	725 – 754
		C-	695 – 724
D	595 – 694	D+	655 – 694
F	0 – 594	D	595 – 654
		F	0 – 594

Note that I reserve the right to change these points totals! Borderline decisions will be based on the Final Exam!

*Grading errors:* For consideration of a possible grading error on an exam or problem set, you must return it to me within one week of the date I hand it back to you. Furthermore, you must include a clear written statement of why you feel you deserve more credit.

#### ***Honor Code:***

This course operates under the guidelines defined by the Millsaps College Honor Code. Unless stated by me, all work turned in for a grade is pledged individual work.

#### ***Homework:***

The solving of spectral problems requires a lot of experience. It is possible that in the beginning you are overwhelmed with the information in each spectrum. To help you I will email you easy problems (if they are not easy for you don't worry, try to solve a few and they get easier with each new, I promise!) that you can work on in groups or alone. Working on these problems will allow you to obtain a "feeling" for that type of spectra. Thus you will work your way up to the level of the problem sets and exams. These

easier problems, in contrast to the problem sets, are not graded and are solely designed to give you practice problems.

### ***Study Groups:***

I encourage you to work with others on the homework and even problem sets, to discuss your work and to compare your answers. Note however, that each student must do all the assigned problems individually! Just copying an answer is unacceptable and will not get you anywhere (In addition, copying is a violation of the Millsaps Honor Code.). Try to learn from others and ask them to explain their reasoning to you. If they truly understand the material they should be able to explain it to others.

As important it is to study in groups: do not lull yourself in a false sense of security just because you were able to “solve” a problem easily in a group. Try to work on them on your own first! If you exam scores are much lower than your problem set scores you should ask yourself if you really solved the problems sets on your own. The problems sets are usually harder than the exams so if you can do them, you should have no problems with the exams!

If after a few weeks you still have a hard time solving spectra come and see me! *I want to help you!*

### ***Changes:***

Changes to this syllabus are not anticipated, but if necessary they will be announced in class and in addition I will send you an email with the change.

## **ACADEMIC HONOR CODE of MILLSAPS COLLEGE**

Millsaps College is an academic community dedicated to the pursuit of scholarly inquiry and intellectual growth. The foundation of this community is a spirit of personal honesty and mutual trust. Through their Honor Code, the students of Millsaps College affirm their adherence to these basic ethical principles.

An Honor Code is not simply a set of rules and procedures governing students' academic conduct. It is an opportunity to put personal responsibility and integrity into action. When students agree to abide by an Honor Code, they liberate themselves to pursue their academic goals in an atmosphere of mutual confidence and respect.

The success of the Code depends on the support of each member of the community. Students and faculty alike commit themselves in their work to the principles of academic honesty. When they become aware of infractions, both students and faculty are obligated to report them to the Honor Council, which is responsible for enforcement.

The pledge signed by all students upon entering the College is as follows:

**As a Millsaps College student, I hereby affirm that I understand the Honor Code and am aware of its implications and of my responsibility to the Code. In the interests of expanding the atmosphere of respect and trust in the College, I promise to uphold the Honor Code and I will not tolerate dishonest behavior in myself or in others.**

Each examination, quiz, or other assignment that is to be graded will carry the written pledge: **"I hereby certify that I have neither given nor received unauthorized aid on this assignment. (Signature)"** The abbreviation "Pledged" followed by the student's signature has the same meaning and may be acceptable on assignments other than final examinations.

It is the responsibility of students and faculty to report offenses to the Honor Code Council in the form of a written report. This account must be signed, the accusation explained in as much detail as possible, and submitted to the Dean of the College.

The Honor Council, 2006-2007

Students:

Maggie Baumgartner, Chair

Rachel Fontenot, Vice-Chair

Joey Quillin, Sergeant-at-Arms

Chris Spear

Elise Diffie

David Butler

Faculty:

Harvey L. Fiser

Mark A Hamon

James E. Bowley, Faculty Secretary

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## *Tentative Lecture and Exam Schedule and Important Date:*

Tuesday, August 29, 10 am, **First class (You made it!!!)**

Wednesday, October 18, 6:30 pm, **Examination**

Tuesday, November 21, 6:30 pm, **Examination**

Tuesday, December 12, 9am, **Final examination**

Week	Topic	Pavia Chapter
1-2	UV/VIS Spectroscopy	7
3-4	CD/ORD Spectroscopy	
5	IR-Spectroscopy	2
<b>6      EXAM 1 (Wednesday, October 18, 6:30 pm)</b>		
-8	IR-Spectroscopy	2
9-11	Mass Spectrometry	8
11-	NMR-Spectroscopy	3-6
<b>11      EXAM 2 (Tuesday, November 21, 6:30 pm)</b>		
-15	NMR-Spectroscopy	3-6
<b>16      FINAL EXAM (Tuesday, December 12, 9 am)</b>		

### *Supplemental Sources of Information on Organic Spectroscopy:*

Below is a very brief list of additional resources you may wish to use. Note that the editions listed here are not necessarily the latest ones and not every book may be available in the library.

#### **A. Books:**

##### *General Spectroscopy:*

Organic Structural Spectroscopy, J.B. Lambert, H.F. Shurvell, D.A. Lightner, R.G. Cooks, Prentice Hall, 1998.

Organic Structure Analysis, P. Crews, J. Rodriguez, M. Jaspars, Oxford, 1998.

Spectra Interpretation of Organic Compounds, E. Pretsch, J.T. Clerc, VCH, 1997.

Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz, Saunders College Publishing, 1996.

Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, McGraw-Hill, 1989.

The Systematic Identification of Organic Compounds, R.L. Shriner, R.C. Fuson, D.Y. Curtin, T.C. Morrill, Wiley, 1980.

##### *NMR Spectroscopy:*

Modern NMR Spectroscopy, J.K.M. Sanders, B.K. Hunter, Oxford, 1997.

High-Resolution NMR Techniques in Organic Chemistry, T.D.W. Claridge, Pergamon, 1999.

Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991.

##### *Mass Spectrometry:*

Interpretation of Mass Spectra, F.W. McLafferty, University Science Books, 1980.

#### **B. Journals:**

Journal of Magnetic Resonance (Academic Press), Magnetic Resonance in Chemistry (Wiley Interscience)

Journal of Mass Spectrometry (Wiley Interscience), Many new compounds and their spectroscopic data are often cited in ACS journals such as: Journal of Organic Chemistry, Journal of the American Chemical Society, Organic Letters

#### **C. Library:**

The library has a vast number of resources. Search for keywords such as NMR, Organic Spectroscopy, Infrared, Mass Spectrometry, etc.

ACS journals: <http://pubs.acs.org/>

Wiley-Interscience journals: <http://www.interscience.wiley.com/>

Elsevier journals (Science-Direct): <http://www.sciencedirect.com/>

Academic Press journals (IDEAL): <http://www.ideallibrary.com/>

#### **D. Internet:**

A variety of web sites dealing with spectroscopy are available free of charge. Three of the better ones are:

Webspectra (UCLA): <http://www.chem.ucla.edu/~webspectra/>

Organic Structure Elucidation (Notre Dame): [http://www.nd.edu/~smithgrp/structure/pbm\\_table.html](http://www.nd.edu/~smithgrp/structure/pbm_table.html)

Integrated Spectral Data Base System for Organic Compounds (Japan): <http://www.aist.go.jp/RIODB/SDBS/menu-e.html>