

CHEM 6115, Spring 2007
ADVANCED ANALYTICAL CHEMISTRY:
MODERN MASS SPECTROMETRY

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6115 Web Page: <http://www.chem.uncc.edu/faculty/cooper/6115/>

Office Hours: By appointment.
Class Meetings: T 5:30–8:20; Burson 118
Exams: Take-home. See lecture outline for dates.
Text: Hoffmann, E. d.; Stroobant, V. *Mass Spectrometry: Principles and Applications* 2nd Ed. (English), New York: Wiley, 2002.
ISBN 0-471-48566-7 (paperback, ~\$65); 0-471-48565-9 (hardcover, out-of-print).
Library: See attached course reserve list. Books may be checked out for three-hour periods.

Grading: EXAM 1	25%
EXAM 2	25%
Special Topic Paper	20%
Special Topic Presentation	5%
FINAL EXAM	25%

Objectives: The discipline of mass spectrometry has enjoyed two distinct renaissance periods. In the first, the serendipitous discovery of organic mass spectrometry from vacuum system contaminants (pump oil) transformed a highly specialized technique for inorganic isotope determination into a broadly applicable technique for routine analysis of relatively nonpolar organic molecules, especially when used as a detector for gas chromatography. More recent advances made since the instructor first entered the field sixteen years ago have again transformed the discipline almost beyond recognition. New “soft” ionization methods for synthetic and biological polymers and for facile mass spectrometric detection of liquid chromatography have dramatically broadened the scope of mass spectrometry and have enabled entirely new approaches to fundamental biology and drug discovery. The tremendous impact of these developments was recognized when the 2002 Nobel Prize in chemistry was awarded in part to two of the pioneers of these techniques. This course seeks to provide a comprehensive overview of analytical mass spectrometry as it is currently practiced, with enough historical background for the student to appreciate fully the present state of the art. Students will learn the fundamentals of ion formation, activation, and fragmentation that underlie the generation of analytically useful mass spectral information. The five basic types of mass analyzers and various means of performing tandem mass spectrometry will be explained in detail. Applications of mass spectrometry to a variety of chemically and biologically related fields will be presented. The course will conclude with each student gaining a more in depth view of a specific aspect or application of mass spectrometry by writing a paper and giving a brief presentation on a topic of personal (or professional) interest.

Exams: There will be two midterm exams and one final. All exams will be given in a take-home format. When working on a take-home exam, you may use *any* resources available to you *except consultation with other people*, including classmates, coworkers, chemistry faculty or staff, or outside experts. The only allowable consultation, whether by email, phone, or in person, is with the instructor; you may not show the exam to anyone else. Any internet or literature sources apart from the text or your course notes should be properly cited. Otherwise, I will assume that all answers you submit represent your own work, written in your own words. Plagiarism or any other form of academic dishonesty (see below) will not be tolerated. You will have one full week to complete each exam, as shown in the attached lecture schedule. The second midterm exam is cumulative: although it will emphasize the material presented after the first exam, knowledge of earlier material may also be assumed or tested. The final exam is comprehensive and will include both specific and “integrative” questions. Each exam is worth 25% of your course grade, and no exam scores will be dropped. Approximate grade breaks will be announced after each exam.

Special Topics: Each student will write a paper on a mass spectrometry-related topic of their choosing, preferably related to their own research or work. A brief outline and statement of topic must be submitted for instructor approval shortly after Spring Break. The paper should explain the purpose, methods, and results of at least one (but preferably three or more) peer-reviewed papers on the topic of interest. Each student will also give a brief (fifteen minute) oral presentation to the class during the final lecture period. The presentation should briefly summarize the topic and explain its significance in the context of the material learned in the course. Further details on preferred format and content will be provided later. The paper is worth 20% of the course grade, the presentation is worth 5%.

Academic Honesty: Students are responsible for knowing and observing the UNC Charlotte Code of Student Academic Integrity (<http://www.legal.uncc.edu/policies/ps-105.html>, or p. 357 of the 2005–2007 Graduate Catalog: <http://www.uncc.edu/gradmiss/GraduateCatalog0507.pdf>).

Prerequisites: A bachelor's or higher degree in chemistry, biology, or a related area, or consent of the instructor.

CHEM 6115: Modern Mass Spectrometry

Spring 2007 Course Outline

Pd	Day / Date	Topics (approximate lecture schedule)	Notes
1	T 9 Jan	Introduction: Mass Spectrometry Terminology	
2	? ? Jan	MS of Volatile Compounds: EI and CI	[Make-up lecture TBA]
3	T 23 Jan	Analytical Information; GC-MS	
4	T 30 Jan	Fragmentation Reaction Mechanisms	
5	T 6 Feb	Mass Analyzers: Time-of-Flight; Quadrupoles	
6	T 13 Feb	Trapping Analyzers: [Quadrupole] Ion Traps; FT-ICR	EXAM 1 distributed
7	T 20 Feb	Sectors; Linked Scans	EXAM 1 collected
8	T 27 Feb	Tandem MS: Ion Activation; Instrumentation	
SPRING BREAK			
9	T 13 Mar	MS of Nonvolatile Analytes: Large Molecule MS	Topic Proposals Due
10	T 20 Mar	Desorption Ionization: FAB, MALDI	
11	T 27 Mar	Electrospray Ionization: LC-MS	EXAM 2 distributed
12	T 3 Apr	Biological MS: Proteins and Peptides	EXAM 2 collected
13	T 10 Apr	Mass Spectrometry and Proteomics	
14	T 17 Apr	Advanced Topics in Protein MS	
15	T 24 Apr	Carbohydrates, Nucleic Acids	
16	T 1 May	Special Topics: Papers Due; In-Class Presentations	FINAL EXAM distributed
	T 8 May	[Official FINAL EXAM Time: 5:00–7:45 pm]	FINAL EXAM collected

Course Reserve Books: The following books will be placed in the Atkins library course reserve. There are many additional mass spectrometry books in our library, but most are out of date. (In particular, books on *biological* mass spectrometry from 1990 or earlier are typically useful only for their historical perspective!) A few newer books were also left off of this list because they are written poorly or at a very low level. Other potentially useful books are available to UNC Charlotte users as on-line “e-books”; I will post links to their catalog entries on the course web page. A list of mass spectrometry journals and other reference materials will also be posted. Course reserve materials may be used in the library for a three-hour period. A few of these books (marked with a ✓) are especially useful; please be considerate of your classmates when using these.

- ✓ CALL NO: QC454 M3 M39 1993
 AUTHOR: McLafferty, Fred W.; Turecek, Frantisek
 TITLE: Interpretation of Mass Spectra, 4th Ed.
 PUB DATA: Sausalito, CA: University Science Books, 1993 (✓ the classic interpretation text!)
- ✓ CALL NO: QD96 M3 S65 1999
 AUTHOR: Smith, R. Martin.; with Kenneth L. Busch., Technical Ed.
 TITLE: Understanding Mass Spectra: A Basic Approach
 PUB DATA: New York: John Wiley, 1999 (✓ applies mainly to chapters 1–4)
- CALL NO: QD272 S6 C43 1985
 AUTHOR: Chapman, John R.
 TITLE: Practical Organic Mass Spectrometry
 PUB DATA: Chichester [West Sussex]; New York: Wiley, 1985 (another classic but less familiar to me)
- CALL NO: QD79 C45 K57 1996
 AUTHOR: Kitson, Fulton G.; Larsen, Barbara S.; McEwen, Charles N.
 TITLE: Gas Chromatography and Mass Spectrometry: A Practical Guide
 PUB DATA: San Diego: Academic Press, 1996 (the best GC-MS book of a weak lot)
- CALL NO: QD96.M3 .B84 2001
 AUTHOR: Budde, William L.
 TITLE: Analytical Mass Spectrometry: Strategies for Environmental and Related Applications
 PUB DATA: Washington, DC: American Chemical Society, 2001 (environmental MS with good GC advice)
- CALL NO: QP519.9 M3 C68 1997
 AUTHOR: Cotter, Robert J.
 TITLE: Time-of-Flight Mass Spectrometry: Instrumentation and Applications in Biological Research
 PUB DATA: Washington, DC: American Chemical Society, 1997 (good book by a TOF pioneer)
- ✓ CALL NO: QP519.9 M3 E44 1997
 AUTHOR: Cole, Richard B., Ed.
 TITLE: Electrospray Ionization Mass Spectrometry: Fundamentals, Instrumentation, and Applications
 PUB DATA: New York: Wiley, 1997 (✓ includes good chapters on mass analyzers)
- CALL NO: QP601 M49 vols. 270-271 (Methods in Enzymology)
 AUTHOR: Karger, Barry L.; Hancock, William S., Eds.
 TITLE: High Resolution Separation and Analysis of Biological Macromolecules, parts A-B
 PUB DATA: San Diego: Academic Press, 1996 (emphasizes separations)
- CALL NO: QP519.9 M3 S58 1996
 AUTHOR: Siuzdak, Gary
 TITLE: Mass Spectrometry for Biotechnology
 PUB DATA: San Diego: Academic Press, 1996 (an easy introduction)
- ✓ CALL NO: QD431.25 A53 S69 2000
 AUTHOR: Snyder, A. Peter
 TITLE: Interpreting Protein Mass Spectra: A Comprehensive Resource
 PUB DATA: New York: Oxford University Press, 2000 (✓ straightforward and practical)
- CALL NO: QP551 M33 2000
 AUTHOR: Chapman, John R., Ed.
 TITLE: Mass Spectrometry of Proteins and Peptides
 PUB DATA: Totowa, NJ: Humana Press, 2000 (more specialized topics)
- CALL NO: QP519.9 M3 M358 2000
 AUTHOR: Burlingame, A. L.; Carr, Steven A.; Baldwin, Michael A., Eds.
 TITLE: Mass Spectrometry in Biology and Medicine
 PUB DATA: Totowa, NJ: Humana Press, 2000 (comprehensive specialized overview)
- CALL NO: QP601 .M49 vol. 402 (Methods in Enzymology)
 AUTHOR: Burlingame, A. L., Ed.
 TITLE: Biological Mass Spectrometry
 PUB DATA: Amsterdam: Elsevier Academic Press, 2005 (recent specialized overview)
- CALL NO: QP601 .M49 vol. 405 (Methods in Enzymology)
 AUTHOR: Burlingame, A. L., Ed.
 TITLE: Mass Spectrometry: Modified Proteins and Glycoconjugates
 PUB DATA: Amsterdam: Elsevier Academic Press, 2005 (more specialized companion to above book)
- CALL NO: QP519.9.M3 D33 2001
 AUTHOR: Dass, Chhabil
 TITLE: Principles and Practice of Biological Mass Spectrometry
 PUB DATA: New York: Wiley, 2001 (comprehensive specialized overview)
- CALL NO: QD96.M3 D69 2004
 AUTHOR: Downard, Kevin
 TITLE: Mass Spectrometry: A Foundation Course
 PUB DATA: Cambridge: Royal Society of Chemistry, 2004 (considered but rejected as a text for this course)