CHEMISTRY 530
Analytical Mass Spectrometry

University at Buffalo | Spring Semester 2017 | Syllabus

STAFF

Instructor:	*Office*	*Office Hours*
Dr. S.J. Ray	410 NSC	By Appointment
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CLASS: M,W,F 10:00AM- 10:50AM Cooke Hall 127A

ABOUT THE COURSE

This course teaches modern analytical mass spectrometry techniques and their application to chemical research. The course will cover basic mass spectrometry fundamentals, instrumentation, experimental methods, and foundational analytical principles. Common types of mass analyzers, ionization sources, detectors, inlet systems, vacuum equipment, data acquisition systems, etc. will be detailed, and the analytical advantages and the fundamental principles which underlie each methodology will be explored. Sophisticated experimental methods, such as tandem mass spectrometry (MS/MS^n) for structural elucidation, and on-line coupling of separations with mass spectrometry (GC/MS, LC/MS, CE/MS, etc.) will also be explored. A portion of the course will be dedicated to mass spectral interpretation. Topics such as isotope distribution and fragmentation patterns (for organic compounds as well as biological compounds) as useful tools in mass spectral interpretation will be covered. Throughout the course, the broad-ranging applications for mass spectrometry will be underscored, from forensics to geological/archaeological dating to biomolecule sequencing to studying atmospheric chemistry. Students must be registered & attend all sessions. Students are responsible for learning material presented regardless of attendance.

LECTURE NOTES: Lecture notes are available in PDF format on the UB Learns website. You are encouraged to download and review the notes before lecture.

TEXT: Mass Spectrometry: Principles and Applications, Edmond de Hoffmann and Vincent Stroobant (Wiley Interscience, 3rd Edition, 2007). This can be purchased at the bookstore or through online vendors, and is available from the UB Library through Ebook Central [Call No. QD96.M3 -- H6413 2007eb]. NOTE: there are a limited number of copies available (online), so access may be limited to off-hours in some cases.

SUGGESTED READING:

Interpretation of Mass Spectra, Fred W. McLafferty and Frantisek Tureek, (Univ. Science Books 1993).
Building Scientific Apparatus, John Moore et al., (Addison-Welsey Co, 1983).
Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation, J. Throck Watson and O. David Sparkman, (Wiley, 2007).
Chemical Ionization Mass Spectrometry, Alex Harrison, (CRC Press, 1983).
Time of Flight Mass Spectrometry: Instrumentation and Applications in Biological Research , Robert J. Cotter, (American Chemical Society Press, 1997).
Mass Spectrometry/Mass Spectrometry: Techniques and Applications of Tandem Mass Spectrometry, Ken Busch, Gary Glish, and Scott McLuckey., (VCH Publishers, 1983).
In addition, a number of paper reprints will be posted on the UB Learns site.

COURSE OUTLINE BY SECTION:

1. Introduction: *Principles, Historical Overview, Terminology.*
2. Analytical Information and Basic Nomenclature: *MS Concepts, MS Experimental Description, Nomenclature, Information Theory, Isotopes, Empirical Formula Determination, Kendrick Mass Defect.*
3. Vacuum Theory and Tools of the Trade: *Kinetic Theory of Gases, Chemical Kinetics, Vacuum Engineering, MS Equipment, Ion Detectors.*
4. Charged-Particle Optics and Computer Simulation (SIMION): *Motion of Ions in Electrostatic and Magnetic Fields, Ion Optics, Common Optical Geometries, An Introduction to SIMION.*
5. Mass Analyzers: *Basic Design, Construction, Operation, and Analytical Capabilities.*
   5A. Time-of-Flight Mass Spectrometers.
   5B. Double Sector (Magnetic and Electromagnetic) Mass Spectrometers.
   5C. Quadrupoles and Quadrupole Ion Traps
   5D: Fourier-Based Instruments: FTICR and Orbitraps.
   5E: Hybrid Instrumentation: Gas Chromatography-Mass Spectrometry (GC/MS), Liquid Chromatography-Mass Spectrometry (LC/MS), Capillary Electrophoresis-Mass Spectrometry (CE/MS).
6. Basic Ionization and Fragmentation Theory and Mechanisms: *Quasi-equilibrium Theory, RRKM Theory, Ionization and Appearance Potentials, Fragmentation Mechanisms.*
7. Introduction to Mass Spectral Interpretation: *Odd and Even-electron ions, 5-step approach to MS interpretation, double-bond equivalent, common ion fragments.*
8. Ionization Sources and MS Interpretation: *Basic Design, Construction, Operation, and Analytical Capabilities.*
   8A: Electron Impact Ionization (EI) and Chemical Ionization (CI).
   8B: Atmospheric-Pressure Chemical Ionization (APCI) & Atmospheric-Pressure Photoionization (APPI).
   8C: Electrospray and Nanospray Ionization (ESI).
   8D: Matrix-Assisted Laser Desorption Ionization (MALDI).
   8E: Atomic Mass Spectrometry.
   8F: Other Ionization Sources: Field Desorption/Ionization (FDI), Fast Atom Bombardment (FAB)/Secondary Ion Mass Spectrometry (SIMS), Ambient Desorption Ionization Mass Spectrometry (ADIMS)
9. Tandem Mass Spectrometry: *Collisionally-Induced Dissociation, Surface-Induced Dissociation, Photo-fragmentation, Mass Spectral Interpretation.*
10. Biomolecular MS Analyses: *Peptides, Proteins, Lipids, Top-down Proteomics, Bottom-Up Proteomics, Spectral Library Search.*
11. Advanced Topics (TBA as permitted):

GRADING *(please consult the UB Learns website for details regarding each graded item)*

MS Problem Sets	5 at 100 pts. each	500 pts.
SIMION Exercise		100 pts.
Midterm Exam		200 pts.
Final Exam		200 pts.
Total		**1000 pts**

The final course grade (A-F including +/–'s) is determined strictly on the basis of the total number of points accumulated. Students should keep all corrected work until they have received their course grade. These are the only materials which will be accepted as evidence of clerical error in determining a course grade.

IMPORTANT DATES. See UB Learns online site for changes to the regular class schedule and exam dates.
LEARNING OUTCOMES. Upon completion of this course, Students will be expected to know the major historical developments in the field of mass spectrometry, the different components of a mass spectrometer, the different types of mass spectrometers and their relative advantages, and the different types of mass common ionization methods and their relative advantages. Students should also develop mass spectral interpretation skills, and develop and understanding of the analytical information available in mass spectra and how mass spectrometry can be used to answer chemical questions.
S**TUDENTS REGISTERED WITH THE OFFICE OF ACCESSIBILITY RESOURCES:** The Chemistry Department works closely with the Office of Accessibility Resources to make it possible for anyone wishing to take a chemistry course to do so. Arrangements must be made well in advance by contacting Accessibility Resources, 25 Capen Hall and Dr. Ray.
ACADEMIC INTEGRITY*:* The University community depends upon shared academic standards. **Academic dishonesty in any form represents a fundamental impairment of these standards.** If, after consultation with the student, an instructor believes the student has committed an act of academic dishonesty, the instructor has the authority to impose sanctions in keeping with this principle. The MINIMUM sanctions to be imposed in Chemistry are as follows:

- First infraction: The maximum point value for the assignment will be subtracted from the student's point total.
- A subsequent infraction: will result in a minimum penalty of subtracting 100 points.

Students should consult the Academic Regulations and Procedures section of the Undergraduate Education Bulletin for a more detailed discussion of possible harsher sanctions and the appeals process.
LATE SUBMISSION OF MATERIALS Due dates will be posted on the UB Learns website and noted on the assignment. Late materials receive a late penalty of 25% one period after the due date and 50% two periods after the due date. Reports will not be accepted after that time.