CHEM 7180 (14923): “MASS SPECTROMETRY: INSTRUMENTATION, ANALYTICAL TECHNIQUES, AND BIOLOGICAL APPLICATIONS”

STAFF

Instructor: Dr. Mary T. Rodgers  
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Office Hours: Monday 2:00 – 3:00 PM; also available other times by appointment

SCHEDULE

Lectures: Mondays, Wednesdays, and Fridays, 12:50 – 1:45 PM  
Location: 0037 State Hall

REQUIRED MATERIALS

2. No other textbooks will be required for this course. Dr. Rodgers will however provide a variety of other handouts, and will also expect you to retrieve your own copy of journal articles available in house or on-line through the WSU library system, make use of other textbooks particularly those on reserve at the Science and Engineering Library, and explore the internet.

Course content will be derived from a variety of sources including but not limited to . . .

2. Various research publications, and in particular, topical mass spectrometry journals
   • Mass Spectrometry Reviews
   • Journal of the American Society for Mass Spectrometry
   • International Journal of Mass Spectrometry
   • Rapid Communications in Mass Spectrometry
   • Journal of Mass Spectrometry
   • European Journal of Mass Spectrometry
   • Organic Mass Spectrometry
   • Journal of the Mass Spectrometry Society of Japan
and other more general chemistry journals such as . . .
   • Journal of the American Chemical Society
   • Analytical Chemistry
   • Journal of Physical Chemistry
   • Physical Chemistry Chemical Physics
   • Accounts of Chemical Research
   • Chemical Reviews
3. Other Mass Spectrometry Text and Reference Books
   - “Mass Spectrometry Principles and Applications”, E. de Hoffmann and V. Stroobant, 2nd edition, John Wiley & Sons Ltd.
   - “Mass Spectrometry”, E. Constantin and A. Schnell, Ellis Horwood Limited
   - “The Principles of Mass Spectrometry as Applied to the Life Sciences”, eds. by Julia Laskin and C. Lifshitz
   - and many more

4. The Internet

Note: WSU faculty and students have electronic access to all of the above mentioned journals as well as a wide variety of other journals at . . .
   http://www.lib.wayne.edu

Of the books listed, several are available in the Science & Engineering library and have been put on reserve for this course. I have requested that the library buy the other books. However, it is only a request and subject to budgetary constraints.
GRADING CRITERIA

Homework Assignments  (30%)

There will be homework assignments approximately every one to two weeks. They will be handed out in class and will be due one week later. Late homework will be subject to a 20% penalty and will be accepted no more than one week late.

All homework is to represent an individual effort. You may discuss the assignments and problems with others, but you must carry out the assignment / solve all of the problems on your own. Feel free to consult with Dr. Rodgers when you have problems.

The nature of the homework assignments will vary during the course and will involve problem solving, descriptive explanations, as well as reading and evaluation of mass spectrometry studies published in the literature, etc.

Midterm Exam  Scheduled during the 3rd or 4th week of October (20%)

There will be an exam approximately midway through the term that will be comprehensive and include all of the material covered in the course up to that point. It is likely to be highly descriptive, but will probably also involve some problem solving as well.

Final Project (25%)

Each student will be required to prepare an oral presentation that will be educational / tutorial in nature and deal with some aspect of mass spectrometry. Appropriate topics for the final project might include but are not limited to: history of mass spectrometry, ionization sources, mass analyzers, ion optics, ion detectors, hyphenated methods, various applications / techniques employed in mass spectrometry studies, … The presentation is not intended to be a mere reporting of mass spectrometry research results.

All students will be required to present their tutorial to the class as an oral presentation.

Final Exam  Monday December 19 at 10:40 AM – 1:10 PM  (25%)

There will be a final exam at the end of the term. It will be comprehensive and examine your understanding of all material / instrumentation / techniques / topics covered in this course. Material covered in the latter part of the course is likely to be emphasized a bit more than material covered before the midterm exam.
COURSE OUTLINE

I. Introduction to Mass Spectrometry
II. History / General Background
III. Qualitative and Quantitative Applications of Mass Spectrometry
IV. Types of Mass Spectrometers
   A. Magnetic (and Electric) Sector Instruments
   B. Quadrupole Mass Spectrometers
   C. Quadrupole Ion Trap Mass Spectrometers
   D. Linear Ion Trap Mass Spectrometers
   E. Time of Flight Mass Spectrometers
   F. Fourier Transform Ion Cyclotron Resonance Mass Spectrometers
   G. Orbitrap Mass Spectrometers
V. Ionization Processes
   A. Electron Ionization (EI)
   B. Photoionization and Photoelectron Spectroscopy (PI, PES)
   C. Chemical Ionization (CI)
   D. Fast Atom/Ion Bombardment (FAB/FIB), Liquid Secondary Ion Mass Spectrometry (LSIMS) and Plasma Desorption
   E. Laser Desorption Ionization (LDI)/Matrix Assisted Laser Desorption Ionization (MALDI)
   F. Thermospray Ionization (TSI), Electrospray Ionization (ESI), and Desorption Electrospray Ionization (DESI)
   G. Coronas, Plasmas, and ArcsElectric / Glow Discharge
   H. Field and Surface Ionization
   I. DART (Direct Analysis in Real Time)
   J. Hybrid Ionization Methods
VI. Ion Activation and Fragmentation Processes
   A. Methods of Ion Activation
      i. Energy Deposition in Electron Ionization and Photoionization
      ii. Activation by Photoexcitation (PD, IRMPD)
      iii. Activation by Blackbody Infrared Radiation (BIRD)
      iv. Ion-Neutral and Ion-Surface Collisional Activation (CAD, CID and SID)
      vi. Ion-Electron and Ion-Ion Interactions (ECD, EDD, ETD)
   B. Ion Fragmentation Mechanisms
   C. Unimolecular Dissociation of Activated Ions
   D. Energy Disposal in Ion Fragmentation Processes
VII. Sample Inlet Systems
VIII. Source / Vacuum Interfaces
IX. Ion Optics
   A. Lens systems
   B. Rf Ion Guides (Quadrupole, Hexapole, Octopole, …)
   C. Rf Ion Funnels
   D. Ion Mobility
COURSE OUTLINE (continued)

X. Detectors
   A. Faraday Cup
   B. Electron Multiplier / Channeltron
   C. Scintillator / Daly Detector
   D. Array and Microchannel Detectors

XI. Sources of Error and Interference

XII. Vacuum Systems
   A. Vacuum Pumps
   B. Design Constraints

XIII. Applications of Mass Spectrometry
   A. Exact Mass Measurements / Elemental Compositions
   B. Isotope Ratios
   C. Structure Determination
   D. Determination of Molecular Properties, Ion Energetics, Chemical Reactivity
   E. Genomics, Proteomics, Glycomics, Metabolomics, . . .
   F. Forensic Applications
   G. Environmental Monitoring and Trace Molecule Detection

COURSE POLICIES

1. ATTENDANCE: Attendance at all lectures and exams is expected in CHM7180. Because the course is intensive and fast-paced, it is important to attend all lectures because they will be the primary mode of communication between Professor Rodgers and the students. In addition, course information and most handouts will be given at the beginning of the lecture. PLEASE AVOID BEING LATE.

2. UNIVERSITY ACADEMIC HONESTY POLICY: Cheating on exams, homework assignments, final projects, and all other forms of dishonest behavior represents a violation of the University Honor Code. All forms of academic dishonesty will be prosecuted to the fullest extent as outlined in the Student Due Process Policy of the University. Any student that commits academic dishonesty will receive a grade of F for the course.

3. HOMEWORK: Late homework will be subject to a 20% penalty and will be accepted no more than one week after it was due. Extensions MAY be granted without penalty in some cases and will be decided upon by Dr. Rodgers on a case by case basis.

4. EXAMS: Excused absences from examinations MAY be granted by Dr. Rodgers, but must be granted BEFORE the starting time of the exam. In cases where Dr. Rodgers approves an absence from an exam, an alternative time for the make-up exam will be chosen by Dr. Rodgers and the student.

5. Please be considerate and respectful of Dr. Rodgers and other students in the course by ensuring that your CELL PHONE IS TURNED OFF PRIOR TO ENTERING THE CLASSROOM FOR LECTURES AND EXAMS.