Syllabus for CHEM 456/556

Mass Spectrometry and Gas-Phase Ion Chemistry, Spring 2022
MWF 11:00 AM, ISC 1061

Instructor: J.C. Poutsma
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Office Hours: by appointment

Text: *Mass Spectrometry. Principles and Applications*, 3rd ed. de Hoffmann and Stroobant. We will also be reading papers from the primary literature.

Grading:

Paper Assignments	20%
Problem Sets	20%
Class Participation	20%
Mid-term presentations	20%
Final paper	20%

Paper Assignments (20%):

During the course of the semester, I will post papers from the current literature on topics that we are covering in the course. You should work on these individually. You should provide a one-page summary of the papers in paragraph format that should include the following:

title of paper and authors with affiliations
statement of the chemical problem that they were addressing
summary of mass spectrometry technique used to address the problem
summary of ancillary techniques used to support the MS
summary of **important** results
summary of conclusions of the paper (did they answer the question or address the problem that they were investigating)
summary of future work motivated
opinion of the paper in terms of style, organization, clarity, significance of the work.

Homework: **(20%)** There will be several problem sets given out over the semester. These will generally be numerical in nature and will cover topics from the course. You may work together on these, but you may also do them individually. Group submissions will all receive the same grade, so choose you groups carefully. The problem sets will be submitted as .pdfs to GradeScope, so you should download the templates from the website. Instructions will be provided when the first assignment is handed out.

Class Participation (20%) Each student will be expected to attend the class prepared to ask questions and participate in discussion. Several papers from the literature will be assigned and discussed in class. Please do not take this class if you do not plan to come to class and participate in discussions.

Mid-Term Presentations (20%) Each student will give two presentations during the semester. They will be group presentations (2 or 3 per group) and each student will speak for 8-10 minutes. The **first** set of presentations will occur around a third of the way through the course and each group should choose a mass spectrometry technique (narrowly defined) and discuss the history of the technique, a brief discussion of the theory behind the technique, and multiple applications of the technique to solve chemical problems. The **second** set of presentations will occur towards the end of the semester and will concentrate on a macro-scale chemical application (broadly defined) and should include multiple examples of different MS-based techniques used to address the problem. Groups will be assigned by me and the groups will change for the two talks. Due to the size of the class, and to try to be equitable, we will have the second set presentations **outside of class either in an evening session or on a weekend afternoon** so that all presentations are in the same session (3.5 to 4 hours).

Final Paper (20%) Each student will write a 6-10 page (double spaced, 11 or 12 point font with appropriate margins) paper on some aspect of mass spectrometry. This paper should be a literature survey and include actual case studies from the current/recent chemical literature. Appropriate topics would include (but are not limited to): a specific ion source and applications, a specific mass analyzer and its applications, a specific application and ms-based approaches to addressing the problem, some combination of these, etc. It is fine to have overlap between your paper and one or more of your presentations. The paper will be graded 50% on content, 25% on grammar and syntax, and 25% in style/presentation. The paper will be due at the end of your final exam period (May 18th at noon).

Extra Assignment for 556: Graduate students will be expected to give an additional 15 minute presentation during the last week of the course on some MS-related topic (which may be the subject of their final paper, but should be on a different topic that the first two presentations).

Tentative Course Outline

Week begin	Topic
January 24	I. Introduction and History of Mass Spectrometry
	A. fundamentals of ion formation
	B. fundamentals of ion interaction
January 31	C. fundamentals of mass analysis
	D. brief history of mass spectrometry
	II. Mass Analyzers
	A. sectors and multi-sector instruments
	B. time of flight and related instruments
February 7	C. quadrupole mass filters
	D. Paul and linear ion traps
	E. FT-ICR
	F.Orbitrap
	III. Sources
	A. electron impact (EI)
	B. chemical ionization (CI)
	C. field ionization (FI)
	D. fast atom bombardment (FAB) and secondary ion mass spectrometry (SIMS)
	E. field desorption (FD)
	F. laser desorption ionization (LDI and MALDI)
February 14	G. atmospheric pressure ionization (API)
	1. electrospray ionization
	2. atmospheric pressure chemical ionization (APCI)
	H. atmospheric pressure SIMS
	1. desorption electrospray ionization (DESI)
	2. direct analysis in real time (DART)
	3. paper spray
	4. others
	I. inductively coupled plasma (ICP)
	III½. Ion Molecule Reactions
	III¾. Detectors
	IV. Tandem Mass Spectrometry
	A. MS-MS in space
	1. basics
	2. modes
	3. activation methods
	4. ion molecule reactions (redux)
	B. MS-MS in time
February 21	C. MS-MS in different specific instruments
	V. EI MS interpretation
	A. ion formation and fragmentation
	1. Lindemann mechanism
	2. quasi-equilibrium theory (QET) and Rice-Ramsperger-Kassel-Marcus (RRKM) theory
	3. ion formation from EI
	4. fundamentals of ion fragmentation
	5. fragmentation rules
	B. Fragmentation Reactions
	1. simple cleavage

	2. rearrangements
February 28	3. functional groups
March 2 - 11	Group Presentations
March 14 - 18	Spring Break
March 21	VI. Proteomics A. introduction B. bottom-up proteomics fundamentals C. bottom-up proteomics applications
March 28	D. top-down proteomics fundamentals and applications VII. Gas-Phase Ion Thermochemistry A. thermochemical quantities B. measurement techniques 1. gas-phase equilibrium 2. bracketing
April 4	3. kinetic method 4. applications VIII. Ion Mobility A. theory
April 11	B. history and development C. instrumentation D. applications IX. Photodissociation and Ion Spectroscopy A. photodissociation introduction B. infrared multiple photon dissociation (IRMPD) C. uv-vis photodissociation D. spectroscopy introduction
April 18	E. IRMPD action spectroscopy F. IR/UV combined spectroscopy G. resonance-enhanced multiple photon ionization (REMPI) and photo-electron spectroscopy (PES) H. blackbody IR spectroscopy (BIRD) X. Hydrogen-Deuterium exchange A. introduction B. gas-phase HDX
April 25	C. solution-phase HDX XI. Isotope Ratio Mass Spectrometry A. Introduction B. stable isotope MS C. radioactive isotope MS
May 2 and 4	Masters Presentations
May 6	XII. eXtreme Mass Spectrometry