

Syllabus for CHEM 456/556  
Mass Spectrometry and Gas-Phase Ion Chemistry, Spring 2019  
Tues, Thurs 11:00 AM, ISC 1111

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Office Hours: by appointment

**Text:** *Mass Spectrometry. Principles and Applications*, 3<sup>rd</sup> ed. de Hoffmann and Stroobant. We will also be reading papers from the primary literature and I will put several general mass spectrometry books on reserve in the chemistry library

**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 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 analytical technique used to address the problem

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.

**Class Participation (20%)** Each student will be expected to attend class prepared to ask questions and participate in discussion. Several papers from the literature will be assigned and discussed in class.

**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 before Spring Break 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 presentation 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.

**Final Paper (20%)** Each student will write a 8-10 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. The paper will be graded 50% on content, 25% on grammar and syntax, and 25% in style/presentation.

**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).

## Tentative Course Outline

- I Introduction and History of Mass Spectrometry
- II. Instrumentation
  - A. Mass Analyzers
    - 1. sectors and multi sector instruments
    - 2. time of flight and related instruments
    - 3. quadrupole mass filters
    - 4. Paul and linear ion traps
    - 5. FT-ICR
    - 6. Orbitrap
    - 7. ion mobility instruments
    - 8. hybrid instruments
  - B. Sources
  - C. Detectors
  - D. Tandem Mass Spectrometry
  - E. QET/RRKM
- III. Interpretation of Mass Spectra
- IV. Gas-Phase Ion Chemistry
  - A. Ion-Molecule reactions
    - 1. reactivity
    - 2. thermochemistry
    - 3. kinetics
  - B. Ion-Ion reactions
  - C. Metal Ion Chemistry and catalysis
  - D. Ion Spectroscopy
- V. Applications
  - A. Proteomics
  - B. Metabolomics
  - C. Forensic Applications
  - D. Stable Isotope chemistry and ICP-MS
  - E. Polymer chemistry.