Chem 2230 – Analytical Spectroscopy
Fall 2019 • Instructor: Professor Sanford A. Asher

In your undergraduate analytical and physical chemistry courses you were exposed to the general principles of measurements and spectroscopic instrumentation. The fundamental atomic and physical properties that one actually measures were probably discussed mostly in your physical chemistry courses, while the measurement and instrumentation issues were discussed in your analytical courses. In Chem 2230, the aim is to develop a more fundamental understanding of spectroscopic processes. We will also focus on some of the key issues in the design of spectroscopic measurements. What is the fundamental process or property to be measured, and why will a particular measurement provide the desired chemical insight? What are the boundary conditions on the measurement? What levels of detection, sensitivity and selectivity are required, and how can they be achieved? What modules (sources, detectors, etc.) should be selected for the measurement? What is the optimum way of doing the experiment (e.g. the time or frequency domain)? Finally, how can the quality of the measurement be assessed, and how can the results be interpreted in terms of chemical processes? A more detailed outline and rough lecture schedule are given on the attached pages.

Class offered: Monday and Wednesdays from 5:30 pm – 6:45 pm, Room 655, Chevron Science Center. The first class is on Monday, August 26 and the last class is on Wednesday, December 11 for the Final Exam. There will be **no class** on Monday, September 2 (Labor Day); Wednesday, October 9; Monday, October 14 and Wednesday, October 16 (Asher Univ. Travel); and Monday, November 25 and Wednesday, November 27 (Thanksgiving Break). Classes resume, Monday, December 2.

Instructor and office hours: Professor Sanford Asher's office is located in Rm. 701 CSC and contact information is: 412-624-8570, email: asher@pitt.edu. Office hours are every Monday from 3:30 pm – 4:20 pm in Rm. 701 CSC or Rm. 706 CSC.
TA and office hours: Mr. Andrew Coukouma's office is located in Rm. 707 CSC and contact information is: 412-624-8875, email: aec85@pitt.edu. Office hours are every Thursday from 2:00 pm – 3:00 pm in Rm. 706 CSC.

Required text: James Ingle and Stanley Crouch, *Spectrochemical Analysis* (Prentice Hall: NJ); and Daniel Harris & Michael Bertolucci, *Symmetry & Spectroscopy* (Dover Publications: NY). A course packet of *Spectrochemical Analysis* can be purchased at the University Bookstore on Fifth Avenue, as the book is no longer in print. Estimated cost of the course packet is ~$64.00. These texts will be supplemented by other required reading materials that will be distributed in class or available on reserve in the Chemistry Library (1st Flr – CSC, Rm. 130). In particular, much of the material in the last half of the course will be based on the current chemical literature. The books on reserve for this course cover a wide range of material, some of which will help you reinforce areas in which your background may be weak, and others which cover material not included (or not covered adequately) in the required text.

Problem sets: Problem sets will be assigned and collected, checked, but not graded in detail. I expect you to do your homework when it is due and your grade depends upon timely performance. Answer keys will be placed on CourseWeb/Blackboard approximately one week after the problem sets are handed out. You are STRONGLY urged to do the problem sets *on your own*, and to refer to the answer keys only after you have given the assignments your best effort.

Grading: There will be three in-class exams, each worth 22.5% of your grade. They will be given on September 30, November 4, and December 11. **Please inform me *immediately* if you have any conflict with these dates.** There will be no make-up exams, but an oral exam will be given if an exam is missed due to serious illness or demonstrated extreme emergency.

Another 22.5% of your grade will be based on a take-home exam about spectroscopic problems described in the chemical literature. Details on this assignment will be distributed early in November. The assignment will be due on December 11. There will be no exceptions.

The remaining 10% of your grade depends upon classroom participation. Some concepts we will cover are difficult. To achieve the intuitive understanding desired, we must discuss the issues and look at them from different view points. Please help! If you don't contribute to the discussion, you will lose points!

Chem 2230: Spectroscopy
Fall 2019

I. **General concepts**

A. Wave, wavevector, polarization (linear, circular)
Refractive index, dielectric constant
Absorption/reflection/refraction
Readings: IC ch 1, 2 (S ch. 7; M pp. 361-419)

B. Beer's law (absorption, scattering) emission
Notation in quantum mechanics
Absorption processes in optical spectroscopy; atomic and molecular energetics
Absorption and emission probabilities (intensities, lifetimes, bandshapes)
Readings: IC ch. 12; (S ch. 13.3, 15.1-15.2, 16.1-16.4, 19.3; M to be assigned)

II. **Experimental approach: aspects of instrumentation**
Readings: IC ch. 3, 4 (S ch. 8,9)

A. Sources
B. Optical elements, monochromators
C. Detectors
D. Noise, the meaning of results, phase sensitive detection, autocorrelation
Readings: IC ch. 5,6, Appendix A; (S ch. 10-12)

Note: The following topics will be among those included in the case studies listed below:

Modulation, interferometry
FT methods, including apodization, digital filtering
Autocorrelation
Phase-sensitive detection
Pump-probe experiments
Hyphenated techniques (special issues for interfacing separation/spectroscopy)

III. **Spectroscopic techniques and applications** *(readings assigned in class)*

A. Atomic absorption: an illustration of concepts
B. UV-Vis absorption (including so-called non-Beer's law issues)
C. IR absorption, including dichroism, sampling interferometry, Fourier Transforms
D. Emission techniques (AE, ICP, fluorescence, phosphorescence, IR)
E. Raman and resonance Raman scattering

Key to readings:

IC: J.D. Ingle, Jr. and S. R. Crouch, Spectrochemical Analysis (Prentice Hall: NY, 1988) (required text)
**NOTE: Spectrochemical Analysis course packet available for purchase in the University Bookstore.*
D.C. Harris & M.D. Bertolucci, Symmetry & Spectroscopy (Dover Publications, NY 1989) (required text).

S: H. A. Strobel and W. R. Heineman, Chemical Instrumentation (3rd ed. Wiley: NY, 1989).

M: A. G. Marshall, Biophysical Chemistry (Wiley: NY, 1978).