

Chemistry 7600 Analytical Spectroscopy (3 Credits)

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General Course Overview

Prerequisites: Although there are no formal prerequisites for this class, student will preferably have taken (or are taking concurrently) most of the following undergraduate courses or their equivalent: undergraduate instrumental (Chem 5640/5650), quantitative analysis (Chem 3000/3005) and physical chemistry (Chem 3060/3070).

This course is intended for chemistry graduate students (Ph.D., MS) or advanced undergraduate or graduate students from a science discipline who meet the above prerequisites. The class will be structured with both formal lectures on the material covered in the attached syllabus as well as a less formal aspect where students will be encouraged to discuss aspects of analytical spectroscopy as it relates to their research problems or general interest areas. Because of the diversity of the material to be covered, there will be no assigned text for the class. Appropriate handouts on particular topics will supplement lectures. Beyond the basic material in the attached syllabus, additional material may be covered in an attempt to accommodate particular interests of students in the class, within the framework of the attached course outline. This may include discussions of specific analytical applications of a particular spectroscopy. The course will be primarily concerned with spectroscopic and mass spectrometric methods applied to organic based compounds, but the basic theory discussed is equally important for all spectroscopic applications. This course will assist the student in implementing various spectroscopies in their individual research areas. It will also provide important fundamental knowledge of spectroscopic methods that should facilitate the future use of analytical spectroscopies in academics or industry.

Grading

Assuming a small class size (5-10 students), grading will be based upon successful completion of the following:

- (a) Two written in-class exams (occurring about week 5 and 10 of the semester).
- (b) A class project as the final exam to be chosen from either:
 - (i) An in class oral presentations (30 minutes) on an approved topic related to spectroscopy that interests you.

Or

- (ii) A written (typed) report on an approved spectroscopy topic (9-12 double spaced pages using a 12-point font).
- (c) Class participation (i.e., regular attendance and interaction).

Course Withdrawal: Students may withdraw from Chemistry 3000 as outlined in the most recent edition of the Utah State University General Catalog (pages 8 & 58).

Additional Provisions: The administration of Chemistry 3000 will adhere strictly to the USU Academic Policies outlined in the 2009-2010 Utah State University General Catalog (pages 80-83). The complete code of Policies and Procedures for Students can also be viewed online at: <http://www.usu.edu/studentservices/studentcode/>

In accordance with the Americans with Disabilities Act, reasonable accommodation will be provided for all persons with disabilities in order to ensure equal participation in Chemistry 3000. A student who requires an accommodation must contact the Instructor. The disability must be documented by the Disability Resource Center. In cooperation with the Disability Resource Center, reasonable accommodation will be provided for students with Disabilities. Course material may be requested in alternate formats through the Disability Resource Center.

Tentative Course Outline

Analytical Spectroscopy Topics

Electronic Spectroscopy

- (1) Fundamental theory relating to Ultraviolet, Visible and Fluorescence Spectroscopy
 - a) Light absorption; light emission, singlet vs. triplet states; measurement aspects of light absorption; forbidden vs. allowed transitions
- (2) UV-Vis molecular chromophores, estimation of UV-Vis absorption wavelength maxima (Woodward-Frieser rules)
- (3) Applications of UV-Vis Spectroscopy

Vibrational Spectroscopy

- (1) Fundamental theory of Fourier transform infrared spectrometry (FTIR) and aspects of data processing
- (2) Instrumental aspects of FTIR and review of optics
- (3) Novel sampling techniques employed in FTIR and computer methods for data analysis
- (4) Fundamental theory of Raman spectroscopy
 - a) Conventional Raman spectroscopy
 - b) FT-Raman spectroscopy
 - c) CCD based Raman spectroscopy
 - d) Surface enhanced Raman spectroscopy
- (5) Applications of Raman spectroscopy

Mass Spectrometry Topics

- (1) Introduction to mass spectrometry (MS)
 - a) Classical mass analyzers including: magnetic/electric sector, quadrupole, ion traps (magnetic and electric sector), time-of-flight
 - b) Newer hybrid instrument designs and the new "orbitrap" mass spectrometer
- (2) "Standard" ionization sources (organic) for MS (EI and CI)
- (3) Ionization techniques for high molecular weight (or thermally labile) molecules
 - a) Early desorption ionization methods (Field Ionization, Field Desorption, SIMS, FAB, plasma desorption, thermospray)
 - b) Electrospray Ionization (ESI) theory and applications
 - c) Matrix-Assisted Laser Desorption/Ionization (MALDI) theory and applications
- (4) MS/MS experiments: collision and photon induced decompositions; new electron capture dissociation (ECD) and electron transfer dissociation (ETD) methods. In-Source and Post-Source Decay in MALDI
- (5) Separation techniques coupled to MS