Chem 249: Syllabus

Experimental Spectroscopy

Winter Quarter 2016
Lecture: TuTh 1100a-1220p Room RH 190

Web Page: http://unicorn.ps.uci.edu/249/

Instructor: Prof. Robert M. Corn

Overview

Chemistry 249 is a graduate level course in Spectroscopy that is offered as part of the graduate analytical program of the Chemistry department. This course is meant to provide graduate students with the information required to (i) understand novel spectroscopic processes and (ii) set up novel spectroscopic experiments. Specifically, in this course students are introduced to the different physicochemical formalisms used to describe the interaction of matter with electromagnetic radiation. In addition, a portion of the class is devoted to the specific example of the vibrational spectroscopy of water. This class is NOT just a survey of different spectroscopic methods, or a primer on how to analyze spectroscopic data to obtain chemical information. A design project at the end of the quarter will test to see how you've assimilated the material.

Course Structure

The course will have a simple structure in which the semester will be divided into four key topic areas of spectroscopic measurement theory. Each section will contain a set of lectures, reading materials, and a problem set.

Topic A. Classical Description of Electromagnetic Radiation

Topic B. Spectral Analysis and the Classical Description of Absorption Susceptibility

Topic C. Basic Quantum Mechanical Models Spectroscopic Systems

Topic D. Semiclassical Description of Absorption: TDPT and Density Matrices as applied to Spectroscopic Processes

Topic E. Vibrational Spectroscopy of Water in the Gas, Liquid and Solid Phase

Problem Sets

With each topic section there will be a problem set to help you sort out the various pieces of information that you receive from the lectures, books, and handouts.

Collaboration on the problem sets is encouraged. Problem sets will be announced in lecture, are available here. Problem Sets MUST be received by the due date for credit. All problem sets are available on the web site:
http://unicorn.ps.uci.edu/249/

Handouts and Reading Materials
Each topic section will include reading from either the recommend text, or supplemental material. All handouts will be posted on the web at:

http://unicorn.ps.uci.edu/243/handouts/handouts.html

Final Project
At the end of the semester, you will put all of your acquired expertise in spectroscopic analysis together to create a document on a particular analysis problem. For more information, please check the web site.

Exams and Grades

The Course will have a total of 600 points. The problem sets will be worth 100 points each, and the Design Project will be worth 100 points. There will be no final exam in this course.

Tentative Course Outline

The five major topic areas have been further subdivided into the following subtopics:

Topic A. Classical Description of Electromagnetic Radiation

1. Maxwell's Equations and Plane Electromagnetic Waves
2. Polarization and Birefringence
3. Fresnel Calculations and Total Internal Reflection
4. Classical Theory of Atomic Absorption

Topic B. Spectral Analysis and the Complex Frequency Dependent Susceptibility

1. LaPlace Transforms and Fourier Transforms
2. Frequency Analysis: Bode and Nyquist Impedance Plots
3. Impedance Spectroscopy

4. Complex Frequency Dependent Susceptibility

Topic C. Basic Quantum Mechanical Models Spectroscopic Systems

1. Spin 1/2 and Two Level Systems (TLS)

2. Simple Harmonic Oscillator (SHO)

3. Atomic Energy Levels and Grotrian Diagrams

4. Perturbation Theory and Level Splittings in Spectroscopy

Topic D. Semiclassical Description of Absorption: TDPT and Density Matrices as applied to Spectroscopic Processes

6. TDPT and Spectroscopic Selection Rules

7. Atomic Absorption: Transition Probabilities, Selection Rules, Term Symbols

8. Density Matrices, T1 and T2, Quantum Molecular Susceptibilities

9. NMR Pulse Sequences and Measuring Relaxation Times

Topic E. Vibrational Spectroscopy of Water in the Gas, Liquid and Solid Phase

10. Local Mode Theory

11. Correlation Functions

12. Hydrogen Bonding

13. Hole Burning

14. Far IR Absorption

Problem Sets and Grading

Each of the course topics will have an associated problem set. The problem sets will include the creation of spreadsheets and some figures -- so please get comfortable with the analysis programs Excel, Igor Pro and Mathematica. Due dates for the problem sets will be announced; no problem sets will be accepted after the due date. Grading for the problem sets will be on an Acceptable/Unacceptable level; an unacceptable problem set

can be converted to an Acceptable one by additional work as prescribed by the instructor on a case by case basis.

The course grade is determined primarily by the problem sets. There are no midterm or final exams in this course. The grade will be based on the number of acceptable problem sets (Don't even THINK about not doing all of problem sets).

Recommended Textbooks

Atomic Spectra and Atomic Structure Gerhard Herzberg
Format: Paperback, 2nd ed., 257pp.
ISBN: 0486601153
Publisher: Dover Publications, Incorporated Pub. Date: November 1987

Title: Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra
Authors: Edgar Bright Wilson, P. C. Cross, J. C. Decius
Format: Paperback, 388pp
ISBN: 048663941X
Publisher: Dover Publications, Incorporated Pub. Date: January 1994

More Recommended Texts:

Molecular Quantum Mechanics
P. W. Atkins and R. S. Friedman
Paperback: 592 pages
Publisher: Oxford University Press, USA; 5 edition (December 30, 2010)
ISBN-10: 0199541426
ISBN-13: 978-0199541423

Quantum Mechanics, Volumes 1 and 2
Claude Cohen-Tannoudji, Bernard Diu, Franck Laloe Format
Paperback: 898 pages
Publisher: Wiley-Interscience; 1 edition (June 1978)
Language: English
ISBN-10: 047116433X
ISBN-13: 978-0471164333
Paperback: 626 pages
Publisher: Wiley; 1 edition (June 1978)
ISBN-10: 0471164356
ISBN-13: 978-0471164357

Title: Quantum Mechanics
Authors: Leonard I. Schiff
ISBN: 0070552878
Format: Hardcover, 544pp
Pub. Date: January 1968

Publisher: McGraw-Hill Companies, The
Edition Number: 3
Recommended E&M Books

Title: Div, Grad, Curl, and All That: An Informal Text on Vector Calculus
Authors: H. M. Schey
ISBN: 0393925161
Format: Paperback, 163pp
Pub. Date: January 2005
Publisher: Norton, W. W. & Company, Inc.
Edition Number: 4

Title: Foundations of Electromagnetic Theory
Authors: John R. Reitz, Frederick J. Milford, Robert W. Christy
ISBN: 0201526247
Format: Hardcover, 630pp
Pub. Date: October 1992
Publisher: Addison-Wesley
Edition Number: 4

Title: Fundamentals of Electromagnetic Phenomena
Authors: Francois Lorrain, Paul Lorrain, Dale R. Corson
ISBN: 0716735687
Format: Hardcover, 600pp
Pub. Date: October 2000
Publisher: W. H. Freeman Company
Edition Number: 1

Title: Electromagnetic Fields and Waves
Authors: Paul Lorrain, Corson, Dale P. Corson
ISBN: 0716718693
Format: Paperback, 754pp
Pub. Date: December 1987
Publisher: W. H. Freeman Company
Edition Number: 3

Title: Quantum Theory of Light
Authors: Rodney Loudon
ISBN: 0198501765
Format: Paperback, 448pp
Pub. Date: November 2000
Publisher: Oxford University Press
Edition Number: 3