

Chemistry 2230: Spectroscopy
Fall 2011 – 3 Credits

Course Information and Syllabus

Instructor: Sunil K. Saxena, 711 Chevron Science Center
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Course Hours and Location: Mon Wed 8:00 am - 9:15 am,

Recommended texts:

“*Symmetry and Spectroscopy*”, Daniel C. Harris and M. D. Bertolucci
This book will be useful for discussing electronic and vibrational spectroscopies.

“*Spin Dynamics: Basics of Nuclear Magnetic Resonance*”, Malcolm Levitt
Class lectures on magnetic resonance will follow the approach used in this book.

Course Goals: To provide you the necessary tools to judiciously integrate the use of various spectroscopic methods in your research.

Course Objectives: Systematically survey spectroscopic methods associated with each part of the electromagnetic spectrum, and gain familiarity with current literature on applications of these techniques to problems in chemistry, physics and biophysics.

Office Hours: To be decided in class.

Course Grading: In class examinations, term-project and project-presentation.

Grades Distribution:

<i>Mid-Term 1: 20 %</i>	<i>Mid-Term 2: 25 %</i>	<i>Mid-term 3: 30 %</i>
<i>Term Project: 15 %</i>	<i>Presentation: 10%</i>	

Exams: There will be three in-class exams during the semester. The first exam will be on **Monday October 3rd** and the second on **Wednesday November 2nd**. Each will be about 75 minutes long. Mid-term 3 is **tentatively** scheduled for November 30th. Coverage for each exam will be outlined in class at least a week before the exam. You will be allowed to bring in a 8.5×11 inch sheet of paper with fundamental constants, parameters, and any key equations or material that you will feel will help in the exam. No make-up exams will be given unless arranged in advance for a serious illness or extreme emergency. Make-up must be taken within a week of the scheduled exams.

Assignments: To aid the study of class material you will be given regular assignments (roughly one every two weeks). You will find that a thorough understanding of each problem set will help you in the examinations. You are encouraged to work collaboratively to solve the problem sets. Assignments will not be graded.

Term Project: You will be asked to choose a research paper and write a term paper on this research. Your paper should identify key technical issues and critically assess the use of a spectroscopic technique within this area. The hope is that this project will allow you to integrate this coursework with your research interests and will serve as a useful resource over the years to come. I expect that you will make several one-on-one appointments with me to help you define and execute your projects.

You should find a paper that focuses on the development of a spectroscopic technique or the application of a spectroscopic technique to solve a chemical or biophysical problem. The paper must be spectroscopy focused. The paper must have been published within the last four years (i.e. from 2006-2010) and must have appeared in one of the following journals: Nature, Science, PNAS, Nature Structural Biology, JACS (only regular articles, no communications). Two students cannot choose the same paper, so it is essential that you meet with me to finalize your choice as soon as you have found an appropriate paper. The deadline for registering your paper with me is Wednesday September 28th. No duplication of term papers will be allowed.

By Monday November 28th, you will submit a final written report. This report will consist of:

- (1) In two lines explain the main achievement of the paper.
- (2) In 5 lines explain the context of the research.
- (3) In 10 lines explain the research methods (you can use up to 2 figures – these will not count towards your 5 line limit)
- (4) In 5 lines explain why this paper was path-breaking or significant.
- (5) In two lines assess the work and suggest future directions

Plagiarism: Your reports will be based on published material but should be demonstrably your own. Each report should encapsulate your understanding of the research material in your own words. You should carefully acknowledge any phrase or idea that is somebody else's. Simply rephrasing someone else's argument is still considered plagiarism. Plagiarism in any form is completely unacceptable in professional science. It is therefore important to give credit where it is due. Ask me if you are unsure of what is and isn't appropriate.

Presentation: You will educate the rest of the class about your paper by giving a short 15-minute oral presentation. Your talk should be targeted to a Pitt graduate student who has not taken this spectroscopy class, i.e. do not assume that your audience is familiar with the subject material.

Students with disabilities who require special accommodations should notify the instructor and the University's Office of Disability Resources & Services (DRS) - 216 William Pitt Union, (412)648-7890/ (412)383-7355 (TTY) - as early as possible in the term. Students may be asked to provide documentation of their disabilities so that DRS may determine the appropriateness of the request. DRS will verify your disability and determine reasonable accommodations for this course.

Syllabus

Introduction to Spectroscopy: Review of Quantum mechanics, Quantization, electromagnetic radiation, interaction of radiation with matter. General Principles of Spectroscopy.

Vibrational Transitions: Vibrational/Rotational levels, transitions, selection rules, IR and Raman Spectroscopy, Instrumentation, Applications.

Electronic Transitions: Molecular Orbitals, Absorptions and UV/Vis Spectroscopy, Fluorescence, Green Fluorescent Proteins, applications to single molecule biophysics and polymer physics. Instrumentation

Transitions between Zeeman Levels: Spins, Zeeman levels, Magnetization and its evolution, detecting magnetic resonance signals, Spectrometer. Relaxation, multiple Pulses, 2D NMR/ESR, Applications: diffusion, Imaging, and dynamics.

Course Schedule

Note: The schedule of lectures is tentative, although every effort will be made to stay on schedule.

Aug 29 (M)	31 (W)
<i>Lecture 1</i> - Syllabus - Introduction to Spectroscopy	<i>Lecture 2</i> - Radiation
Sep 7 (W)	12 (M)
<i>Lecture 3</i> - Review of Quantum Mechanics	<i>Lecture 4</i> - Quantization of Energy levels
14 (W)	19 (M)
<i>Lecture 5</i> - Interaction of Radiation with matter	<i>Lecture 6</i> - Selection Rules, Einstein Coefficients, populations
21 (W)	26 (M)
<i>Lecture 7</i> - Diatomics-Electronic and Vibrational levels	<i>Lecture 8</i> - anharmonic oscillators
28 (W)	Oct 3 (M)
<i>Lecture 9</i> - Many atom molecules, Raman	Midterm Exam 1
5 (W)	11 (T)
<i>Lecture 10</i> - Molecular Orbitals, Spin	<i>Lecture 11</i> - Electronic Transitions
12 (W)	17 (M)
<i>Lecture 12</i> -Fate of the Excited state/FRET	<i>Lecture 13</i> - Spins, precession, magnetization

Oct 19 (W)	24 (M)
<i>Lecture 14</i> - CW and FT experiments	<i>Lecture 15</i> - Operators in Matrix Form, Energy level (TE)
26 (W)	31 (M)
<i>Lecture 16</i> - Effect of Pulse, Instrumentation	<i>Lecture 17</i> - Midterm Exam 2
Nov 2 (W)	7 (M)
- Spins, magnetization, T_1	<i>Lecture 18</i> - Spins in a magnetic field, precession <i>Lecture 19</i>
9 (W)	14 (M)
<i>Lecture 20</i> - RF pulses, MR Spectrometer	<i>Lecture 21</i> - NMR Spin Interactions
16 (W)	21 (M)
<i>Lecture 22</i> - ESR Spin Interactions	<i>Lecture 23</i> - ESR/NMR selection rules
28 (M)	30 (W)
<i>Lecture 24</i> - Special Topics	- Midterm Exam 3
Dec 5 (M)	7 (W)
<i>Lecture 25</i> - Special Topics	<i>Lecture 26</i> - Special Topics
12 (M)	
<i>Lecture 27</i> - Special Topics	