

# Chem 564    Molecular Spectroscopy    Course Outline Fall 2014

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Textbook: *Molecular Spectroscopy* by Jeanne L. McHale (optional)  
Advance copies of revised chapters of *Molecular Spectroscopy*, 2<sup>nd</sup> edition, will be provided.

Class will be held in Todd 411, Tuesday and Thursday from 12:00 noon to 1:15 pm.

I prefer open office hours rather than scheduled times, but please email me first to confirm my availability. Or just drop in and see if I am available.

## Overview

This course is designed to present the tools and concepts needed to understand how light-matter interactions can be applied to uncover the structure and dynamics of molecules from interpretation of gas-phase and condensed-phase spectroscopy experiments. Emphasis is placed on the quantum mechanical fundamentals of modern spectroscopic techniques that exploit the microwave, infrared, visible and ultraviolet regions of the electromagnetic spectrum. At the end of the semester, students will know how to select and interpret a variety of experimental tools that are available to chemists, physicists and materials scientists.

## Prerequisites

Previous study of quantum mechanics, preferably at the graduate level, is critical to success in the class. It is also hoped that students have previously studied group theory. Appendix C from the first edition of *Molecular Spectroscopy* provides an overview of Group Theory that can bring the student up to speed with respect to the skills needed for this class.

## Course Materials

The course will be taught from the author's own textbook *Molecular Spectroscopy* which is currently available at the bookstore. I am working on a second edition and will provide chapter copies throughout the semester. If you wish to have a complete book you may want to purchase a copy, but it is not required. As I am in the midst of revising Chapters 1 through 12 and writing two new chapters (Chapter 13, Nonlinear Optical Spectroscopy and Ch. 13 Time-resolved Spectroscopy), I appreciate your input into the revised chapters including new homework problems.

## Approximate Schedule of Lecture Topics

<u>Date</u>	<u>Topic</u>
T Aug 26	Introduction and Course Overview, Ch. 1 Review of Quantum Chemistry
Th Aug 28	Ch. 2 Electromagnetic Radiation
T Sept 2	
Th Sept 4	Ch. 3 Electric and Magnetic Properties of Matter
T Sept 9	
Th Sept 11	Ch. 4 Time-Dependent Perturbation Theory
T Sept 16	
Th Sept 18	Ch. 5 Time-Dependent Approach to Spectroscopy (selected highlights of this chapter will be covered)
T Sept 23	Ch. 6 Experimental Considerations
Th Sept 25	
T Sept 30	Ch. 7 Atomic Spectroscopy
Th Oct 2	
T Oct 7	First Midterm (in-class)
Th Oct 9	Ch. 8 Rotational Spectroscopy
T Oct 14	
Th Oct 16	
T Oct 21	Ch. 9 Vibrational Spectroscopy of Diatomics
Th Oct 23	
T Oct 28	
Th Oct 30	Ch. 10 Vibrational Spectroscopy of Polyatomics
T Nov 4	
Th Nov 6	
T Nov 11	No Class
Th Nov 13	Ch. 11 Electronic Spectroscopy
T Nov 18	
Th Nov 20	Second Midterm due (take-home)
T Nov 25	No Class
Th Nov 27	No Class
T Dec 2	
Th Dec 4	Ch. 12 Raman Spectroscopy
T Dec 9	
Th Dec 11	

If time permits, brief overviews of new chapters, Ch. 13 Nonlinear Optics and Ch. 14 Time-resolved Spectroscopy, will be included.

T Dec 16      FINAL EXAM      8:00 – 10:00 AM

## Grading

Grades are based on regular homeworks, two midterms and one two-part final exam. The homeworks will be assigned at least one week before the due date, and no late homeworks will be accepted unless special arrangements are made with the instructor. Students are permitted to work together on homeworks and may also seek the instructors help, but direct copying of one another's homeworks will be penalized by assigning a grade of zero. Exams, on the other hand, must be worked individually, whether take-home or in-class, and the penalty for cheating on exams will be to receive a grade of F for the course.

The final exam will consist of two parts, a take-home part due on Dec. 16, and a qualitative in-class final exam. The take-home part will be more mathematical in nature and the in-class part will consist of conceptual questions (non-mathematical) that will test your mastery of basic concepts of spectroscopic techniques to determine structure and dynamics of molecules.

### *Grading Scheme*

Homeworks (scaled to)	200
Two Midterms @ 100	200
<u>Final Exam</u>	<u>200</u>
	600

86 – 100%	A
60 – 85%	B
40 – 59%	C

### *Students with Disabilities*

Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; 509-335-3417) to schedule an appointment with an Access Advisor. All accommodations must be approved through the Access Center. For more information contact a Disability Specialist