

Chemistry 882: Spectroscopy and Kinetics

Spring 2005 MWF, 1:50 p.m. – 2:40 p.m., Room 136

<http://poohbah.chem.msu.edu/courses/CEM882/cem882.htm>

Instructor

Dr. David Weliky

Room 41 Chemistry

355-9715 ext. 281

weliky@chemistry.msu.edu

Office Hours: To be announced

Prerequisite: One semester of undergraduate quantum mechanics

Textbook: P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, Third Edition

Optional books

P. W. Atkins, Quanta, Second Edition

P. W. Atkins and R. S. Friedman, Solutions Manual for Molecular Quantum Mechanics

James R. Barrante, Applied Mathematics for Physical Chemistry

For the kinetics section of the course, I will be lecturing mostly from J. Steinfeld, J. S. Francisco, and W. L. Hase, Chemical Kinetics and Dynamics, D. Voet and J. G. Voet, Biochemistry, and D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach. However, much of the material can be found in any undergraduate physical chemistry text.

Reference Books (on reserve in BPS Library)

1. Peter F. Bernath, Spectroscopy of Atoms and Molecules
2. C. H. Townes and A. L. Schawlow, Microwave Spectroscopy
3. Gerhard Herzberg, Molecular Spectra and Molecular Structure (vols. 1-4)
4. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics and Solutions Manual
5. Claude Cohen-Tannoudji, Bernard Diu, Franck Laloe, Quantum Mechanics (vols. 1,2)
6. Jack D. Graybeal, Molecular Spectroscopy
7. Donald A. McQuarrie and John D. Simon, Physical Chemistry: A Molecular Approach
8. Thomas C. Farrar and Edwin D. Becker, Pulse and Fourier Transform NMR
9. Charles P. Slichter, Principles of Magnetic Resonance
10. James R. Barrante, Applied Mathematics for Physical Chemistry
11. P. W. Atkins, Quanta: A Handbook of Concepts
12. Jeffrey Steinfeld, Joseph S. Francisco, and William L. Hase, Chemical Kinetics and Dynamics
13. Donald Voet and Judith G. Voet, Biochemistry

Course Homepage: <http://poohbah.chem.msu.edu/courses/CEM882/cem882.htm>

Course notes, homework problem sets, homework and exam solution sets, and course announcements can be found on the course homepage.

Syllabus (approximate)

Week	Topic	Reading
Jan. 10 – 14	Orders of Magnitude of Atoms and Molecules	A&F, Introduction and Orientation; 7.3 McQuarrie&Simon, 1–8
Jan. 19 – 21	Quantum Mechanical Background	A&F, Chapter 1 through 1.20
Jan. 24 – 28	Vibrational Spectroscopy	A&F, Harmonic Oscillator, 2.16 – 2.18; 10.8 – 10.10; Further Information, 6, 7
Jan. 31 – Feb. 4	Rotational Spectroscopy	A&F, Chapter 3 through 3.8; 10.2 – 10.5, 10.11; Further Information 9
Feb. 7 – 11	Electronic Spectroscopy	A&F, 3.9 – 3.14; Chapter 7 through 7.2; Further Information 8
Feb. 14 – 25	Magnetic Resonance Spectroscopy/ Matrix Approaches to Quantum Mechanical Problems	A&F, Further Information, 22, 23; McQuarrie&Simon, 14-1 to 14-6; Barrante, Chapters 8 and 9
Feb. 28 – Mar. 4	Perturbation Theory	A&F, 6.1 – 6.5, 6.8
Mar. 14 – 25	Radiative Transitions and Lineshapes	A&F, 6.11 – 6.18; 10.1 Further Information 16, 17
Mar. 28 – Apr. 8	Introduction to Kinetics/Rate Laws	Steinfeld, Chapter 1; McQuarrie&Simon, 28-1 to 28-7
Apr. 11 – 15	Transition State Theory/Complex Reaction Mechanisms	Voet, Chapter 13.1; Steinfeld, Chapter 2.3; McQuarrie&Simon, 29-1 to 29-7
Apr. 18 – 22	Catalysis and Enzymes	Voet, Chapter 13.2 – 13.3
Apr. 25 – 29	Atmospheric Kinetics	Steinfeld, Chapter 15

Homework

There will be five homework assignments in the course. They are due in class on the given due dates. Late homework assignments will not be accepted. You are permitted to work with your classmates on solving the problems but what you hand in should not be a direct copy of other students' work.

Homework #1: Orders of Magnitude of Atoms and Molecules/Quantum Mechanical Background
Due Wednesday, Feb. 2 in class

Homework #2: Vibrational Spectroscopy/Rotational Spectroscopy/Electronic Spectroscopy
Due Wednesday, Feb. 23 in class

Homework #3: Magnetic Resonance Spectroscopy/Matrix Approaches to Quantum Mechanical Problems
Due Wednesday, Mar. 16 in class

Homework #4: Perturbation Theory/Radiative Transitions and Lineshapes
Due Monday, Apr. 4 in class

Homework #5: Introduction to Kinetics/Rate Laws and Transition State Theory/Complex Reaction Mechanisms
Due Monday, Apr. 25 in class

Exams

There will be three exams in the course.

The first exam will cover: Orders of Magnitude of Atoms and Molecules, Quantum Mechanical Background, Vibrational Spectroscopy, Rotational Spectroscopy, and Electronic Spectroscopy. It will be given sometime during the weeks of Feb. 21 – Mar. 4.

The second exam will cover: Magnetic Resonance Spectroscopy/Matrix Approaches to Quantum Mechanical Problems, Perturbation Theory, and Radiative Transitions and Lineshapes. It will be given sometime during the weeks of Apr. 4 – Apr. 15.

The third exam will cover: Introduction to Kinetics/Rate Laws, Transition State Theory and Complex Reaction Mechanisms, Catalysis and Enzymes, and Atmospheric Kinetics. It will be given during the Final Exam time, Monday, May 3, 12:45 p.m. – 2:45 p.m.

A review sheet will be prepared for each exam. In addition, formulas and constants will be provided on the exam, unless the exam question explicitly asks you to derive them. You will also be permitted to bring in two pages to each exam with any information which you think is important.

I expect to see all of your work for problems on homework and exams. You may receive partial credit when you do have written work and reasoning, but an incorrect answer. Typically, you will not receive any credit for a correct answer with no written work or reasoning.

Grading

A final grade will be calculated using the following percentages.

Homework: 34%
Exam #1: 22%
Exam #2: 22%
Exam #3: 22%

The homework portion of your grade will be calculated from the following percentage:

$$(\text{Number of points which you received} / \text{Total possible number of points}) \times 100$$

For each exam, your grade will be calculated from the following percentage:

$$(\text{Number of points which you received} / \text{Total possible number of points}) \times 100$$

The anticipated final grading scale is:

4.0	80% – 100%
3.5	70% – 80%
3.0	60% – 70%
2.5	50% – 60%
2.0	40% – 50%
1.5	30% – 40%
1.0	20% – 30%
0.0	0% – 20%