

CHEM 461
(Introduction to) QUANTUM MECHANICS and SPECTROSCOPY
(a.k.a. “Quantum Mechanics” or “P-Chem 1”)
Meeting: MWF 1:00 – 1:50 pm (Neckers 218)
FALL 2006

Professor Boyd M. Goodson
Department of Chemistry and Biochemistry
Office: Neckers 113
Phone: x3-6427
Email: bgoodson@chem.siu.edu

I. Office Hours:
TBA

II. Grading:

20%	Homework (approximately 8-10 assignments, but we'll see)
10%	<i>Classroom Participation</i> (see below)
20%	1 st Midterm
20%	2 nd Midterm
30%	Final Exam

III. Textbooks, etc.
Levine, *Quantum Chemistry* (5th Ed.) (primary text)
Atkins and de Paula, *Physical Chemistry* (8th Ed.)

Various other sources can also be helpful and/or interesting:

Lower-level texts:

Warren S. Warren, *The Physical Basis of Chemistry* (2nd Ed.)
David Ball, *Physical Chemistry*

Higher-level texts/references:

Messiah, *Quantum Mechanics*
J.J. Sakurai, *Modern Quantum Mechanics*
Claude Cohen-Tannoudji, Bernard Diu, Frank Laloe, Bernard Dui, *Quantum Mechanics*
(scores of others)

Other texts: Philosophy of Quantum Mechanics, “popsci” books, etc.:

Bernard D'Espagnat, *Veiled Reality: An Analysis of Present-Day Quantum Mechanical Concepts*
J. Polkinghorne, *The Quantum World*
Bas van Fraassen, *Quantum Mechanics: An Empiricist View*
David Z. Albert, *Quantum Mechanics and Experience*

IV. **Class Philosophy and Content**

We will mostly follow a “traditional” course in how we cover the relevant aspects of physical chemistry (quantum mechanics, then spectroscopy). Much of what we cover will at least loosely follow the introduction of topics taken from the primary text—but I will try to “deepen” things a bit right from the start. Problem sets will contain questions I write, along with some from various textbooks. Despite whatever you have taken (or remember), I will do my best to start the class assuming as little knowledge as possible—but we may go very deeply, very quickly!

The following concepts will (likely) be covered, not necessarily in order (and sometimes simultaneously):

- (1) Review of Mathematical and Physical Background
(and why we need it)
- (2) Beginning History (the “ultraviolet catastrophe”, et al.)
- (3) Principles of quantum mechanics
Wave motion and the Schroedinger Equation(s)
Heisenberg Uncertainty Principle
Postulates of Quantum Mechanics
- (4) Model Systems
Free Particles, Particle in a box, Harmonic Oscillator, Morse Oscillator, etc.
- (5) Angular Momentum (orbital, spin)
- (6) Approximation Methods (Perturbation Theory and Variational Theory)
- (7) Atomic Structure and Spectroscopy
- (8) Pauli Principle
- (9) Born-Oppenheimer Approximation
- (10) Introduction to Effects of Symmetry (Group Theory)
- (11) Introduction to Molecular Spectroscopy (e.g., vibrational, rotational, electronic, NMR)
- (12) Introduction to Statistical Mechanics (maybe)

V. **Helpful Hints**

- (1) Classroom participation—by you—is critical. For one thing, I have made it 10% of the grade. It is important that you not only show up, but that you contribute by asking questions, giving answers, working out board-problems, **stumping the Prof.**, helping your classmates, etc. Because of the nature of the material (particularly how it involves the application of very abstract ideas), you will all learn much faster if the class is highly interactive. This will also help me discern how well the material is being integrated into your brains. *COME TO CLASS EXPECTING TO BE ASKED QUESTIONS AND TO WORK PROBLEMS.*
- (2) Keep Up. A great deal of the course’s material is cumulative, so don’t fall behind. If you find yourself falling behind, get help—nip it in the bud.

- (3) Ask Questions. If something isn't clear, let me know. Chances are, someone else (perhaps the Prof.) is having trouble with it too. If people don't speak up, I will assume that a concept is understood by all.
- (4) Do the Problem Sets. Success in this class will take Practice, Practice, Practice. You have my permission to work on Problem Sets in groups, but don't mindlessly "Team Xerox" anything. I advise you to work on them separately as best you can, and then work together to solve the harder problems.
- (5) Beat this stuff into your head repeatedly. I have found that "quantum-mechanical masochism" can be a useful substitute for raw brilliance. There is no question that some of this stuff is really hard to absorb—much less "understand". Approach this material with an appropriate sense of wonder—but also be prepared to "go to war" with it—and don't let it win!

VI. Basic Class Schedule (tentative)

Week of (Monday):

Aug. 21	MEET M, W, F
Aug. 28	MEET M, W, F
Sept. 4	(No Meeting on Labor Day); MEET W, F
Sept. 11	MEET M, W, F
Sept. 18	MEET M, W, F
Sept. 25	MEET M, W, F
Oct. 2	MEET M, W, F; On Friday, First Midterm Exam (In Class)
Oct. 9	MEET M, W, F
Oct. 16	MEET M, W, F
Oct. 23	MEET M, W, F
Oct. 30	MEET M, W, F
Nov. 6	MEET M, W (<i>perhaps no meeting on Veteran's Day, don't know</i>)
Nov. 13	MEET M, W, F; On Friday, Second Midterm Exam (In Class)
Nov. 20	<i>No Meeting all week; THANKSGIVING BREAK</i>
Nov. 27	MEET M, W, F
Dec. 4	MEET M, W, F
Dec. 11	FINALS WEEK; Date, Time of Final TBA