

# Chemistry 341 – Quantum Chemistry and Spectroscopy

(note: new name from past years!)

## Fall 2009 - Professor Samet

Office – Stuart 1107

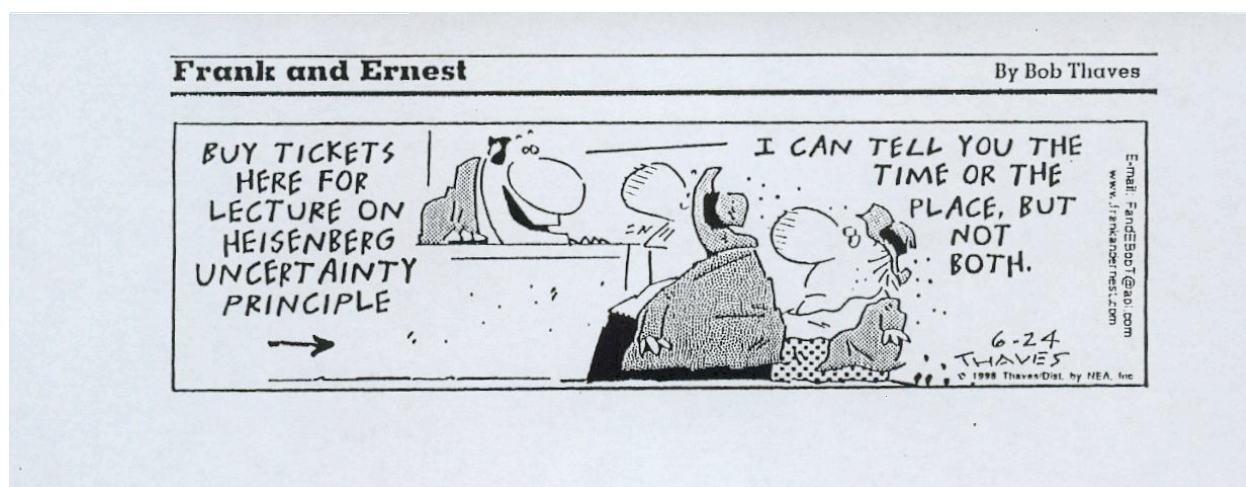
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*and by appointment.*

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*“Quantum Mechanics provides the fundamental underpinning of all modern science. The equations describe the behavior of very small objects – generally speaking, the size of atoms or smaller – and they provide the ONLY understanding of the world of the very small. Without these equations, [scientists] would be unable to design working nuclear power stations, build lasers, or explain how the sun stays hot. Without quantum mechanics, chemistry would still be in the Dark Ages, and there would be no science of molecular biology – no understanding of DNA, no genetic engineering – at all.*

*-from In Search of Schrodinger's Cat: Quantum Physics and Reality, John Gribbin.*

*“Anyone who is not shocked by quantum theory has not understood it.”*

*-Neils Bohr (1885-1962)*

**CHEM 341**  
**QUANTUM CHEMISTRY AND SPECTROSCOPY**  
**M, W, F 10:30-11:20**  
**Stuart Hall, Room 1113**

**FALL 2009**  
**Prof. Cindy Samet**

### **A. Nature of Course**

This course deals with the study of individual atoms and molecules from the viewpoint of quantum mechanics (rather than dealing with the properties of bulk matter from the viewpoint of thermodynamics). Quantum mechanics is the study of the nuclei and electrons that make up atoms and molecules. Mechanics is the science of motion. The pioneers in physical science in the seventeenth century believed that motion of objects is the primary property of matter and that all other properties can be explained in terms of mechanics. Newton's Laws are the basic axioms of classical mechanics. These laws, which you should have encountered in Physics, formed the basis of physical science until the end of the nineteenth century. Despite its success in many areas, classical mechanics could not explain the nature of the chemical bond or of intermolecular forces. The emergence of quantum mechanics, also called wave mechanics, changed this dramatically during what is sometimes referred to as "the thirty years that shook physics". Much of our present understanding of molecular structure and properties depends on quantum theory. In fact, many of the calculations done "behind the scenes" in molecular modeling programs (such as Spartan, which we have in our chemistry modeling lab) involve quantum mechanics and the Schrodinger Equation.

We will begin by examining some important experiments that paved the way for the emergence of quantum theory. We will then study various types of motion, relating the quantum mechanics of the motion to energy and structure. Our aim is to see how the quantum theory provides a coherent explanation for the phenomenon of spectroscopy, which is central to a complete understanding of chemistry. Although the quantum theory is rather abstract and mathematical (since we are studying things our eyes cannot see), it is a necessary prerequisite to the study of spectroscopy, which is an indispensable tool for the chemist. It is through the use of spectroscopy that chemists "see" atoms and molecules, and thereby learn about their structures. The primary goal of this course is to learn just enough about quantum mechanics to enable us to gain a thorough understanding of how spectroscopy works.

The material will be pitched at such a level as to require calculus. However, the calculus required is very basic and was covered in Calculus I and II, which are prerequisites for this course. Physics 111 or 131, or concurrent enrollment, is also a prerequisite for this course. If you have any questions about these prerequisites, or have not yet taken physics, please see me. The only chemistry prerequisite for this course is Foundations of Chemistry (141).

### **B. Course Objectives**

This course covers three main areas, each with specific objectives, which are listed below each main topic:

## **Quantum Mechanics and Atomic Structure**

1. Understand the postulates of quantum mechanics
2. Apply quantum mechanics to the study of atomic structure

## **The Chemical Bond**

3. Apply quantum mechanics to the study of molecular structure
4. Understand the role of symmetry in quantum mechanics

## **Foundations of Chemical Spectroscopy**

5. Understand the use of spectroscopy in the study of atoms and molecules
6. Understand the relationship between quantum mechanics and spectroscopy.

\*note: As you will see from the course schedule, these three areas will not be studied separately but will be intermingled so the important connections and interrelationships are well understood.

In addition, we will address the big picture:

## **The Real World**

7. Apply spectroscopy (experimental) and modeling (theoretical), which are both applied quantum mechanics, to real word problems.

## **C. Text**

The primary text is *Physical Chemistry Volume 2: Quantum Chemistry, Spectroscopy, and Statistical Thermodynamics* by Peter Atkins and Julio de Paula. Note well: This book is a subset of the full text by the same authors, titled Physical Chemistry. It is much less expensive, paperback, and therefore much easier to bring to class. This represents an exciting new change, which means we use the entire textbook, rather than just about a third.

The secondary required reading is: *In Search of Schrodinger's Cat: Quantum Physics and Reality* by John Gribbin (Bantam Books, 1984)

\*\*\*note well: it is imperative that you bring your textbook to class!!! I often refer to figures and diagrams from the text, and it will help you immensely to have the book in front of you!

## **D. Grading**

Grades will be based on a total of 1000 points as follows:

<u>Description</u>	<u>Points:</u>
Three 1-hour exams (150 each)	450
Four problem sets	250

Quantum Mechanics Essay (Gribbin)	100
Final Exam	200

**Exams:** There will be three 1-hour exams and a comprehensive final exam in this course. The semester exams will be given during the normal class period. There will be a cumulative final exam – made up of an in-class portion and a take-home portion, which will be due at the time of the in-class final exam. This will be explained thoroughly in class. There will be NO MAKEUP EXAMS!!! If you miss an exam, your grade on the final exam will replace your zero. *In all cases, your grade on the final exam may replace one of your exam grades that is lower than your grade on the final exam.* If something unusual happens that causes you to miss a second exam, we will work something out on a case-by-case basis depending upon the situation.

**Problem sets:** There will be 4 graded problem sets, which, together, comprise a significant portion (one fourth) your course grade. These problem sets give us a chance to solve problems that are not appropriate for exams, but which are very important to understand and can help to solidify the concepts. You will be allowed to ***work with your classmates from this current class*** on these problem sets. This will provide you with an opportunity to do what scientists do – to collaborate and discuss the material. After working with classmates, however, ***it will be up to you to write your own, final draft of the problem set. The work you turn in must be your own, and you must provide an explanation and show all work clearly.*** *Be sure to list those students you worked with on your problem set.* Also, I ask that you ***do not consult with anyone who took this course previously or any professors other than myself.*** Finally, on some of the problem sets I will include an opportunity for extra credit points to be earned for solving an especially involved problem.

**Gribbin Essay:** Early in the semester, you will receive an assignment to write a quantum mechanics essay. You are to write this essay *on your own, without consulting anyone but me.* A separate document on this assignment will be posted on Bb, and the assignment will be discussed in detail in class. The essay will be due on the last day of classes. The main focus of the essay will be the following question: *How does quantum mechanics change our view of the world from that of classical mechanics?* We will discuss the many ways in which this essay can be addressed.

**Academic Conduct:** For this course, the definition of plagiarism is that found in Dickinson College's policy for academic conduct, as outlined in the *Dickinson College Community Standards* ([www.dickinson.edu/students/code.html](http://www.dickinson.edu/students/code.html)). While I encourage you to get together with classmates and discuss the class notes and material and to collaborate on the problem sets, I trust that you are mature enough to follow instructions carefully and to *work individually on an assignment when that is what is required for that particular assignment.* If you have any questions, feel free to ask me!

**Attendance:** Please don't miss class unless you absolutely cannot make it. Although I do not have a formal attendance policy, it is extremely important to be in class. Many of the concepts in this course are not easy to grasp from a textbook alone, and therefore your grade will most likely reflect your attendance. If you miss class excessively, I reserve the right to lower your overall

course grade (by one letter grade, for example). I consider three absences to be excessive, since at that point you have missed an entire week of the semester, and at this point it is likely that your grade will be affected.

**Note: All problem set due dates and exam dates are noted on the course calendar. Announcements will also be posted on Blackboard. I reserve the right to make adjustments to this schedule.**

**A final note about the course:** During the semester, you will be working on problem sets and keeping up with new material. All of the work is QUITE DO-ABLE IF YOU KEEP THE SCHEDULE IN MIND. I have taken much time to plan the schedule that follows. PLEASE USE IT!

**\*\*\*All course information will be posted on Blackboard, and it will be essential for you to check Blackboard on a daily basis for announcements, etc.**

**NOTE: COURSE SCHEDULE IS A SEPARATE DOCUMENT.**