CHEMISTRY 1140

PHYSICAL CHEMISTRY: QUANTUM CHEMISTRY

Professor Richard M. Stratt

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Lecture

Mon Wed Fri 10:00-10:50 am GeoChem 351

Office Hours

Mon, Weds 2:00-3:00 pm Thurs 1:30-2:30 pm (plus by appointment)

Required Textbook

D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach* (University Science Books, Sausalito, CA, 1997)

Some other places to go for additional reading

D. A. McQuarrie, *Quantum Chemistry* (University Science Books, Mill Valley 1983).

P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 3rd. ed. (Oxford University Press, Oxford, 1997).

I. N. Levine, *Quantum Chemistry*, 5th ed. (Prentice Hall, Upper Saddle River, NJ, 2000).

M. A. Ratner and G. C. Schatz, *Introduction to Quantum Mechanics in Chemistry* (Prentice Hall, Upper Saddle River, NJ, 2001).

Homework

Roughly one problem set every week. Problem sets count significantly towards the grade.

Examinations

One one-hour examination in class + One three-hour final exam. All exams are open book, open notes.

OUTLINE

I. *Introduction*

II. *Classical Waves and the Wave Equation*

III. *The Wave Function and the Schrodinger Equation*

The Quantum Mechanical Wave Equation
Probability Concepts
The Particle in a Box
The Uncertainty Principle
Chemical Bonding (take 1)

IV. *The Mathematical Stuff That Makes Quantum Mechanics Work*

Operators
Expectation Values, Commutators, and Matrices
Chemical Bonding (take 2)

V. *Harmonic Oscillators and Vibration*

Classical and Quantum Mechanics of Vibration
Spectroscopy

VI. *Three Dimensions and Angular Momentum*

Rigid Rotors and the H Atom

VII. *Many-Electron Systems*

Pauli Exclusion Principle
Atomic and Molecular Electronic Structure.