# CHEMISTRY 163A

MWF 9:30-9:10 **Fall 2002**
Thimann Lecture 1

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TEXT: *Quantum Chemistry*, D. A. McQuarrie

ON RESERVE:
1. *Quantum Chemistry*, D. A. McQuarrie, QD462.M26
2. *Physical Chemistry, a Molecular Approach*, D. A. McQuarrie and J. D. Simon, QD453.2.M394
2. *Atoms and Molecules*, M. Karplus, QD461.K33
3. *Quantum Chemistry*, J. P. Lowe, QD462.L69
4. *Physical Chemistry*, P. W. Atkins, QD453.2, A88 1994b

DISCUSSION SECTIONS:
M 5:00-6:00 P.M., Thimann 101
M 6:15-7:25 P.M., Thimann 101
Tu 2:00-3:10 P.M., Thimann 101
W 8:00-9:10 A.M, Thimann 101

TUTORIAL: Tu 7:00-9:00 P.M., Thimann 391

MATHEMATICAL/PHILOSOPHICAL ENRICHMENT: W 2:00-3:10 P.M., Thimann 391

GOOD WWW SITES FOR INTRODUCTORY QUANTUM CHEMISTRY:

Chemistry 163A WWW:
**http://www.chemistry.ucsc.edu/teaching/switkes/CHEM160A/Fall02**

**or http://www.chemistry.ucsc.edu/ ✦ course pages**

(class handouts, course information, question-answer bulletin board and links to additional sites)

C. David Sherrill at Georgia Tech:
http://vergil.chemistry.gatech.edu/notes/quantrev/quantrev.html

Reproduction of WWW material from [the late] Prof. Kent Wilson, UC San Diego
http://www.chemistry.ucsc.edu/teaching/switkes/CHEM163A/Fall02/KWILSON/qm/qm.html

TO BE COVERED (note exam dates!):

I. Origins of quantum mechanics (Ch. 1)

A. Observations that didn't fit classical theories
1. Stern-Gerlach experiments
2. Photoelectric effect
3. Compton scattering
4. Davisson-Germer experiment
5. Existence of the hydrogen atom (Rutherford Model)

B. New "laws" from the quantum conspirators

1. Energy of light waves "quantized"
2. Particles have wavelength
3. Bohr model of the hydrogen atom
4. Indeterminacy Principle

II. Foundations of quantum mechanics

A. Some new mathematical vocabulary (Ch. 2)

B. Postulates of quantum mechanics (Ch. 4)

III. Application of quantum mechanics to model systems and implications of the results

A. Confined particles with kinetic energy (Ch. 3)
1. Solutions of Schrödinger equation
2. Why only certain energies?
3. Calculation and meaning of average or observable values

B. Harmonic oscillator—a model for molecular vibrations (Ch. 5)

1. Setting up the Schrödinger equation and separation of CM and relative motions
2. Methods of solution
3. Energies and nature of the wave functions (why only certain energies?)
4. Tunneling—a purely quantum phenomenon
5. The harmonic oscillator and the vibration of diatomic molecules

**MIDTERM ABOUT HERE — THURS., 31ST OCTOBER (EVENING)**

D. The rigid-rotor—a model for molecular rotation (Ch. 6, pp. 203-221)

1. Schrödinger equations in many dimensions.
2. Separation of variables technique

3. Solutions of the $\Theta$ and $\Phi$ equations (relationships to atomic s, p, d, .... orbitals)

4. Energy levels and rotational spectra
5. Rotational angular momentum

IV. The hydrogen atom (Ch. 6, pp. 221-243)

A. Hamiltonian and solution techniques

B. Energies and wavelength

C. Interpretation of the *n, l, m,* $m_S$ quantum numbers

D. Shapes, "signs," and modal properties of hydrogenic orbitals

V. Many electron atoms (Ch. 7-8)

A. Approximate methods

B. Screening and orbital energies

C. Spon and Pauli exclusion principle

D. Term Values and Russell-Saunders coupling

VI. Bonding in molecules (Ch. 9)

A. Molecular orbitals and LCAO method

B. Implications of m.o.'s for $H_2$
1. Energy
2. Electron density distribution
3. The "electron pair bond"

C. Homonuclear diatomic molecules
1. M.O. energy ordering
2. Prediction of molecular properties

D. Polyatomic molecules
Delocalized orbitals

VII. Spectroscopy (Survey of Ch. 10, detailed presentation of in Chemistry 163C)

A. General principles

B. Vibrational spectroscopy

C. Electronic spectroscopy

D. Qualitative survey of various types of chemical and biochemical spectroscopy

**FINAL EXAM — WEDNESDAY, 4 DECEMBER, 4:00-7:00 P.M.**