Chemistry 461/881 Lecture Topics Fall 2000

Text: PHYSICAL CHEMISTRY A Molecular Approach

McQuarrie and Simon

A. Historically Significant Experiments (Chapter 1)

Blackbody Radiation

Photoelectric effect

Compton effect

DeBroglie Wavelength

Atomic spectra are not continuous (line spectra)

Heisenberg Uncertainty Principle

B. Particle on a line/in a box (Chapter 3)

Model

Classical expectations

Time dependent Schrodinger equation

Time independent Schrodinger equation

Wavefunction

Eigenvalue equation

Hamiltonian operator

Linear operator

Solution to time independent Schrodinger equation

Boundary conditions

Stationary states

Energy levels

Quantum number

Wavefunctions

Orthogonality

Normalization

Probability interpretation

Correspondence principle

Expectation values

Uncertainty principle

General time dependent solution

C. Particle in a plane/particle in a two dimensional box (not in text)

Time independent Schrodinger equation

Boundary conditions

Separability

Energy levels

Degeneracy

Wavefunctions

Orthogonality

Symmetry

Probability interpretation

General time dependent solution

D. Particle in a cube (Chapter 3)

Time independent Schrodinger equation

Boundary conditions

Separability

Energy levels

Degeneracy

Wavefunctions

Orthogonality

Symmetry

Probability interpretation

General time dependent solution

E. Harmonic oscillator (Chapter 5)

Model

Classical expectations

Time dependent Schrodinger equation

Time independent Schrodinger equation

Eigenvalue equation

Hamiltonian operator

Linear operator

Solution to time independent Schrodinger equation

Boundary conditions

Stationary states

Energy levels

Quantum number

Wavefunctions

Orthogonality

Normalization

Probability interpretation

Correspondence principle

Expectation values

Uncertainty principle

General time dependent solution

Diatomic molecules

F. Postulates & Principles of Quantum Mechanics (Chapter 4)

Postulate 1

Postulate 2

Postulate 3

Postulate 4

Postulate 5

Commuting operators

G. Rigid Rotor (Chapter 5)

Classical motion

Spherical coordinates

Moment of inertia

Angular momentum

Schrodinger equation

Separation of variables

Wavefunctions

Spherical harmonics

Energy levels

Linear molecules

Rotational spectroscopy

H. Hydrogen atom (Chapter 6)

Model

Time independent Schrodinger equation

Separation of variables

Energy levels

Degeneracy

Wavefunctions

Radial functions

Angular functions

s,p,d,f,g,…functions

Probability density

Radial distribution function

Contour surfaces

I. Approximation methods (Chapter 7)

Variation method

Trial function

Boundary conditions

Linear variation function

Secular determinant

Perturbation theory

J. Multielectron atoms (Chapter 8)

Atomic units

Hamiltonian Operator

Variational calculations on He atom

Electron spin

Hartree-Fock equations

Correlation energy

Antisymmetry principle

Slater determinants

Term symbols

Coupling of angular momenta

Equivalent versus non-equivalent electrons

Hund's rules

K. Chemical bond & diatomic molecules (Chapter 9)

Born-Oppenheimer approximation

Schrodinger hamiltonian

Linear combination of atomic orbitals for H_2^+

Binding energy of H_2^+

Electronic configuration of first row diatomics

Photoelectron spectra

Heteronuclear diatomics

L. Bonding in polyatomic molecules (Chapter 10)

sp, sp^2, sp^3, Hybrid orbitals

Photoelectron spectra

Huckel theory

M. Molecular spectroscopy (Chapter 13)

Electromagnetic spectrum & molecular processes

Diatomic molecules

Rotation-vibration spectroscopy

Rotational spectroscopy

Anharmonicity in vibrational spectroscopy

Excited electronic states

Electronic spectra

N. Polyatomic molecules

Rotational spectra

Vibrational spectra / normal modes

Electronic spectra

Selection rules

O. Nuclear magnetic resonance spectroscopy (Chapter 14)

Nuclear spin

Nuclear magnetic moments

Energy levels for Nucleus in a magnetic field

Resonance condition

Chemical shifts

Spin-spin coupling

P. Lasers (Chapter 15)

Electronic relaxation processes

Dynamics of absorption and emission

Two level system

Three level system

Population inversion

Generic structure of a laser

Helium-neon laser