

Chemistry 483 Lecture Topics Fall 2009

Text

PHYSICAL CHEMISTRY A Molecular Approach

McQuarrie and Simon

A. Background (M&S, Chapter 1)

Blackbody Radiation

Photoelectric effect

DeBroglie Wavelength

Atomic spectra are not continuous (line spectra)

Bohr model of the atom

Heisenberg Uncertainty Principle

B. Particle on a line (M&S, Chapter 3) and on the circumference of a circle (not in text)

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 two dimensional rectangular and circular 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 (M&S, Chapter 3)

Time independent Schrodinger equation

Boundary conditions

Separability

Energy levels

Degeneracy

Wavefunctions

Orthogonality

Symmetry

Probability interpretation

General time dependent solution

E. Harmonic oscillator (M&S, 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 and vibrational spectroscopy

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

Postulate 1

Postulate 2

Postulate 3

Postulate 4

Postulate 5

Commuting operators

G. Rigid Rotor (M&S, 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 (M&S, 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

iii. Mathematics review (M&S, Chapter E)

Determinants

I. Approximation methods (Chapter 7)

Variation method

Trial function

Boundary conditions

Linear variation function

Secular determinant

Perturbation theory

J. Multielectron atoms (M&S, 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 (M&S, 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 (M&S, Chapter 10)

sp, sp², sp³, Hybrid orbitals

Photoelectron spectra

Huckel theory

M. Group Theory and Symmetry (M&S, Chapter 12)

Symmetry elements

Groups

Group multiplication table

Matrix representations

Character tables

N. Molecular spectroscopy (M&S, Chapter 13)

Electromagnetic spectrum & molecular processes

Diatomic molecules

Rotation-vibration spectroscopy

Selection rules

Rotational spectroscopy

Anharmonicity in vibrational spectroscopy

Excited electronic states

Electronic spectra

Normal modes

O: Nuclear Magnetic Resonance Spectroscopy (M&S, Chapter 14)

Nuclear Spin

Magnetic moments

Proton MNR

Chemical shifts

Spin-Spin coupling

First order spectra

Second order spectra

P: Lasers, Laser Spectroscopy and Photochemistry (M&S, Chapter 15)

Relaxation mechanism

Rate of electronic transitions

Population inversion

Structure of a Laser

Photochemical applications