

# CONTENTS

## CHAPTER

### I. INTRODUCTION: THE OLD QUANTUM THEORY

The Composition of Matter, 1. Black-Body Radiation, 1. The Photoelectric Effect, 2. Bohr's Theory of the Hydrogen Spectrum, 3. The Old Quantum Theory, 5. The Dual Nature of Light, 6. The Dual Nature of Electrons, 7.

### II. THE PRINCIPLES OF CLASSICAL MECHANICS

Generalized Coordinates, 8. Lagrange's Equations, 9. Generalized Momenta and Hamilton's Equations, 14. Vibration Theory and Normal Coordinates, 16.

### III. THE PRINCIPLES OF QUANTUM MECHANICS

The Uncertainty Principle, 21. Wave Mechanics, 23. Functions and Operators, 25. The General Formulation of Quantum Mechanics, 27. Expansion Theorems, 31. Eigenfunctions of Commuting Operators, 34. The Hamiltonian Operator, 37. Angular Momenta, 39.

### IV. THE DIFFERENTIAL EQUATIONS OF QUANTUM MECHANICS

The Linear Differential Equation of the Second Order, 48. The Legendre Polynomials, 52. The Associated Legendre Polynomials, 52. The General Solution of the Associated Legendre Equation, 53. The Functions  $\Theta_{l,m}(\theta)$  and  $Y_{l,m}(\theta, \varphi)$ , 57. Recursion Formulae for the Legendre Polynomials, 59. The Hermite Polynomials, 60. The Laguerre Polynomials, 63.

### V. THE QUANTUM MECHANICS OF SOME SIMPLE SYSTEMS

The Free Particle, 68. The Particle in a Box, 70. The Rigid Rotator, 72. The Rigid Rotator in a Plane, 75. The Harmonic Oscillator, 75.

### VI. THE HYDROGEN ATOM

The Hydrogen Atom, 80. Hydrogenlike Atoms, 84. Some Properties of the Wave Functions of Hydrogen, 85. The Continuous Spectrum of Hydrogen, 90.

### VII. APPROXIMATE METHODS

Perturbation Theory, 92. Perturbation Theory for Degenerate Systems, 96. The Variation Method, 99. The Ground State of the Helium Atom, 101.

### VIII. TIME-DEPENDENT PERTURBATIONS: RADIATION THEORY

Time-Dependent Perturbations, 107. The Wave Equation for a System of Charged Particles under the Influence of an External Electric or Magnetic Field, 108. Induced Emission and Absorption of Radiation, 110. The Einstein Transition Probabilities, 114. Selection Rules for the Hydrogen Atom, 116. Selection Rules for the Harmonic Oscillator, 117. Polarizability; Rayleigh and Raman Scattering, 118.

### IX. ATOMIC STRUCTURE

The Hypothesis of Electron Spin, 124. Electronic States of Complex Atoms, 128. The Pauli Exclusion Principle, 129. The Calculation of Energy Levels, 132. Angular Momenta, 133. Multiplet Structure, 135. Calculation of the Energy Matrix, 143. Fine Structure, 151. The Vector Model of the Atom, 155. Selection Rules for Complex Atoms, 159. The Radial Portion of the Atomic Orbitals, 162. The Hartree Method, 163. The Periodic System of the Elements, 167.

### X. GROUP THEORY

Matrices, 172. The General Principles of Group Theory, 175. Group Theory and Quantum Mechanics, 184. The Direct Product, 187.

# CONTENTS

## CHAPTER

### XI. ELECTRONIC STATES OF DIATOMIC MOLECULES

Separation of Electronic and Nuclear Motions, 190. Molecular Orbitals; The  $H_2^+$  Ion, 192. The Electronic States of the  $H_2^+$  Ion, 201. Homonuclear Diatomic Molecules, 203. Heteronuclear Diatomic Molecules, 208.

### XII. THE COVALENT BOND

The Hydrogen Molecule, 212. The Covalent or Electron-Pair Bond, 218. The Quantitative Treatment of  $H_2O$ , 225. The General Theory of Directed Valence, 227.

### XIII. RESONANCE AND THE STRUCTURE OF COMPLEX MOLECULES

Spin Theory and Bond Eigenfunctions, 232. Evaluation of the Integrals, 240. The Two-Electron Problem, 244. The Four-Electron Problem, 245. The Concept of Resonance, 248. The Resonance Energy of Benzene, 249. The Resonance Energy of Benzene by the Molecular Orbitals Method, 254.

### XIV. THE PRINCIPLES OF MOLECULAR SPECTROSCOPY

Diatomic Molecules (Spin Neglected), 258. Symmetry Properties of the Wave Functions, 261. Selection Rules for Optical Transitions in Diatomic Molecules, 262. The Influence of Nuclear Spin, 265. The Vibrational and Rotational Energy Levels of Diatomic Molecules, 268. The Vibrational Spectra of Polyatomic Molecules, 273.

### XV. ELEMENTS OF QUANTUM STATISTICAL MECHANICS

The Maxwell-Boltzmann Statistics, 282. The Fermi-Dirac Statistics, 285. The Bose-Einstein Statistics, 287. Relation of Statistical Mechanics to Thermodynamics, 289. Approximate Molecular Partition Functions, 292. An Alternative Formulation of the Distribution Law, 296.

### XVI. THE QUANTUM MECHANICAL THEORY OF REACTION RATES

Formulation of the General Theory, 299. General Behavior of the Transmission Coefficient, 311. Transition Probabilities in Non-Adiabatic Reactions, 326. Thermodynamics of Reaction Rates and the Effect of Applied External Forces, 330.

### XVII. ELECTRIC AND MAGNETIC PHENOMENA

Moments Induced by an Electromagnetic Field, 332. Dipole Moments and Dielectric Constant, 337. The Theory of Optical Rotatory Power, 342. Diamagnetism and Paramagnetism, 347.

### VIII. SPECIAL TOPICS

Van der Waals' Forces, 351. The Quantum-Mechanical Virial Theorem, 355. The Restricted Rotator, 358.

## APPENDIX

I. Physical Constants, 361.

I. Vector Notation, 361.

III. The Operator  $\nabla^2$  in Generalized Coordinates, 363.

IV. Determinants and the Solution of Simultaneous Linear Equations, 368.

V. The Expansion of  $\frac{1}{r_{ij}}$ , 369.

VI. Proof of the Orthogonality Relations, 371.

VII. Symmetry Groups and their Character Tables, 376.

III. Some Special Integrals, 388.

IX. General References, 389.