



# ***contents***

***guide to major figures***      *ix*

***guide to major tables***      *xiii*

***preface***      *xv*

## ***1 electromagnetic radiation and photons***

- 1.1** The Electromagnetic Wave Theory of Radiation      *1*
- 1.2** Light Scattering      *14*
- 1.3** Interference and Diffraction      *20*
- 1.4** Blackbody Radiation      *24*
- 1.5** The Photoelectric Effect, Compton Scattering, and  
Photoelectron Spectroscopy      *28*
  - Problems      *32*
  - References      *37*

## **2      *the nature of matter***

2.1	Classical Mechanics and Rotational Kinetic Energy	39
2.2	The Classical Interaction of a Charged Particle with an Electric Field	46
2.3	Vibrational Motion and Lagrange's Equations	52
2.4	Hamilton's Equations	58
	Problems	63
	References	66

## **3      *quantum theory***

3.1	Early Quantum Theory of Atoms	68
3.2	Wave-Particle Duality, the Wave Equation, Wave Packets, and Uncertainty	71
3.3	The Postulates of Quantum Mechanics	75
3.4	Time-Independent Perturbation Theory	89
3.5	The Variation Method for Any State and the Secular Equation	95
3.6	Probability and Time-Dependence	98
3.7	Time-Dependent Perturbation Theory and the Semiclassical Interaction Between Radiation and Matter	103
	Problems	116
	References	118

## **4      *model quantum mechanical problems***

4.1	Particle-in-a-Ring	120
4.2	Internal Rotation	128
4.3	Nonrelativistic Description of the Hydrogen-like Atom	135
4.4	The Angular Solution and the Spherical Harmonics	138
4.5	Angular Momentum	140
4.6	Solution of the Radial Equation, Hydrogen-like Atom Energies, and the Radial Distribution	142
4.7	Notation, Linear Transformations, Hybrid Orbitals, and Spherical Harmonic Selection Rules	147
4.8	Electron Spin and the Spin-Orbit Interaction	153
4.9	The Electronic and Nuclear Zeeman Effect in the Absence of Orbital Electronic Angular Momentum: ESR	163
4.10	The Nuclear Zeeman Effect in the Absence of Electronic Angular Momentum: NMR	175
4.11	The Rigid Rotor	184
4.12	The Harmonic Oscillator and Normal Coordinates	214
	Problems	233
	References	263

## **5      *atomic theory and atoms in solids and molecules***

5.1	Atomic Orbitals with Application to the Helium Atom	265
5.2	The Hartree-Fock Self-Consistent Field (SCF) Atomic Orbitals and Analytical Approximations	269

5.3	Configuration Interaction (CI)	283
5.4	Angular Momentum in Atoms	285
5.5	The Spin-Orbit Interaction in Alkali Atoms, $j$ - $j$ Coupling, and Pair Coupling	290
5.6	Nuclear-Electronic Magnetic Interactions	296
5.7	Atoms and Crystal Field Theory	299
5.8	Nuclear Quadrupole Interactions	310
5.9	Atoms in the Solid State	315
	Problems	322
	References	328

## 6 *the electronic structure of molecules*

6.1	The General Hamiltonian, Separation of Coordinates, and the Force Theorems	331
6.2	LCAO-MO in Diatomic Molecules	338
6.3	<i>ab initio</i> Calculations of the Electronic Structure of Molecules; LCAO-MO-SCF and LCAO-MO-SCF-CI	347
6.4	Valence Bond Theory	359
6.5	Approximate LCAO-MO-SCF Theories	363
6.6	The Extended Hückel Theory and Molecular Charge Distribution	367
6.7	The Simple $\pi$ -Electron Hückel Theory	372
6.8	Magnetic Interactions in Molecules in the Absence of Nuclear Spins	380
6.9	Nuclear Magnetic Shielding and Nuclear Spin-Rotation Interactions	392
6.10	Electric Field-Dependent Electronic Interactions and Molecular Polarizability	402
	Problems	412
	References	418

## 7 *molecular spectroscopy*

7.1	Molecular Absorption Spectroscopy	423
7.2	The Doppler Effect and Convolutions	432
7.3	Heisenberg's Representation of the Absorption of Electromagnetic Energy and Correlation Functions	437
7.4	The Bloch Equations, Steady-State Solutions, Power Saturation, and Molecular Relaxation	444
7.5	Double-Resonance Saturation Effects	464
7.6	Transient Effects, Fourier Transform Spectroscopy, and Multiple Pulse Experiments	468
7.7	Interferometers, Lasers, Picosecond Pulses, and More Fourier Transform Spectroscopy	482
	Problems	491
	References	493

## 8 *electromagnetic scattering*

8.1	Introduction	496
8.2	Rayleigh and Raman Scattering in Gases, Kinetic Theory, and Rotational Quenching	505

8.3	Isotropic Rayleigh and Brillouin Scattering in Dense Gases and Pure Liquids	515
8.4	Anisotropic Rayleigh and Raman and Isotropic Raman Scattering in Liquids: Translational and Rotational Diffusion	527
8.5	X-Ray Scattering; Free Atoms, Free Molecules, Condensed Phases, and Low-Angle Scattering	539
8.6	Concentration Fluctuations and Electric Field Effects	557
	Problems	566
	References	569

## 9 *the scattering of particles*

9.1	Classical Scattering	572
9.2	Quantum Mechanical Scattering; Wave Packets	585
9.3	Quantum Mechanical Scattering; Plane Waves	588
9.4	Quantum Mechanical Scattering; Partial Waves	594
9.5	Elastic Electron Scattering from Atoms	607
9.6	Elastic Electron Scattering from Molecules; Electron Diffraction	613
	Problems	619
	References	621

## *appendix*

A.	Units, Constants, and Conversion Factors	625
B.	Mathematical Miscellany	634
	B.1 Matrices, Vectors, and Dyadics	634
	B.2 Fourier Transforms	641
	B.3 Dirac Delta Functions	644
C.	Differential Equations	646
	C.1 Associated Legendre Polynomials	646
	C.2 Associated Laguerre Polynomials	649
	C.3 Hermite Polynomials	651
D.	Numerical Methods	653
	D.1 Orthogonalization Methods	653
	D.2 Symmetric Orthogonalization	654
	D.3 Schmidt Orthogonalization	655
	D.4 The Method of Least Squares	656
E.	Symmetry and Group Theory	658
	E.1 Molecular Symmetry and Groups	658
	E.2 Matrix Representation and Character Tables	660
	E.3 Normal Coordinate Symmetry and the Symmetry of Vibrational Wavefunctions	672
	E.4 Construction of Hybrid Orbitals	677
	E.5 Quantum Mechanics and Matrix Element Theorems	678
F.	General References	681
	References in Appendix	681

## *index* 683