

CONTENTS

The principles of quantum mechanics

1. Introduction	1
2. The wave function	5
3. The Bohr atom	11
4. Stationary states and the particle in a box	14
5. The color of conjugated organic molecules	19
6. Operators and their properties	22
7. Approximate methods in quantum mechanics	28
Problems	34
Bibliography	35

2 Exact solutions of the Schrödinger equation

1. Introduction	37
2. The harmonic oscillator	38
3. Vibration of diatomic molecules, an example	45
4. The rigid rotor	48
✓ 5. Angular momentum	55
✓ 6. The hydrogen atom	63
✓ 7. Properties of the eigenvalues and eigenfunctions of the hydrogen atom	72
Problems	83
Bibliography	85

3 Atomic structure

1. Introduction	87
2. Calculations on the He atom	96
3. The electron spin	102
4. Exclusion principle and spin	109
5. Atomic orbitals	114
Problems	120
Bibliography	121

4 Light and spectroscopy

1. The nature of light	123
2. Transition probabilities	131
3. Transition probabilities and quantum theory	135
4. The maser and the laser	139
Problems	143
Bibliography	144

5 The spectra of diatomic molecules

1. Experimental information	145
* 2. The Born-Oppenheimer approximation	150
3. The vibrational motion of a diatomic molecule	158
4. Molecular symmetry	166
* 5. Selection rules and spectral intensities in electronic bands	169
6. Intensities in the infrared and microwave regions	182
Problems	183
Bibliography	185

6 The chemical bond

1. Introduction	187
2. The hydrogen molecular ion	189
* 3. The hydrogen molecule	196
4. Diatomic molecules	202
5. Electronegativity	212
* 6. Hybridization	216

7. Unsaturated molecules	227
8. Conjugated and aromatic molecules	232
Appendix	244
Problems	246
Bibliography	248
7 The solid state	
1. Crystal structures	249
2. Ionic crystals	252
3. Metals and semiconductors	255
4. Molecular crystals	265
Problems	270
Bibliography	271
8 Magnetic resonance	
1. Introduction	273
* 2. Relaxation phenomena	279
* 3. Chemical shifts	286
* 4. Spin-spin coupling	290
* 5. Electron spin resonance	300
Problems	306
Bibliography	307
Index	309