

Contents

Preface		v
I <u>Electrons</u> in Atoms		1
1-1	Introductory Remarks	1
1-2	Bohr Theory of the Hydrogen Atom (1913)	1
1-3	The Spectrum of the Hydrogen Atom	5
1-4	The Need to Modify the Bohr Theory	9
1-5	Electron Waves	9
1-6	The Uncertainty Principle	11
1-7	The Wave Function	12
1-8	The Schrödinger Wave Equation	13
1-9	The Normalization Constant	13
1-10	The Radial Part of the Wave Function	13
1-11	The Angular Part of the Wave Function	14
1-12	Orbitals	14
1-13	Electron Spin	17
1-14	The Theory of Many-Electron Atoms	20
1-15	Russell-Saunders Terms	22
1-16	Ionization Potentials	27
1-17	Electron Affinities	33
II <u>Diatoms</u> Molecules		36
2-1	Covalent Bonding	36
2-2	Molecular-Orbital Theory	38

2-3	Bonding and Antibonding Molecular Orbitals	39
2-4	Molecular-Orbital Energy Levels	42
2-5	The Hydrogen Molecule	46
2-6	Bond Lengths of H_2^+ and H_2	47
2-7	Bond Energies of H_2^+ and H_2	47
2-8	Properties of H_2^+ and H_2 in a Magnetic Field	48
2-9	Second-Row Homonuclear Diatomic Molecules	49
2-10	Other A_2 Molecules	58
2-11	Term Symbols for Linear Molecules	60
2-12	Heteronuclear Diatomic Molecules	62
2-13	Molecular-Orbital Energy-Level Scheme for LiH	67
2-14	Ground State of LiH	68
2-15	Dipole Moments	69
2-16	Electronegativity	69
2-17	Ionic Bonding	73
2-18	Simple Ionic Model for the Alkali Halides	75
2-19	General AB Molecules	78

III Linear Triatomic Molecules

3-1	BeH_2	
3-2	Energy Levels for BeH_2	89
3-3	Valence-Bond Theory for BeH_2	93
3-4	Linear Triatomic Molecules with π Bonding	95
3-5	Bond Properties of CO_2	100
3-6	Ionic Triatomic Molecules: The Alkaline Earth Halides	

IV Trigonal-Planar Molecules

4-1	BF_3	106
4-2	σ Molecular Orbitals	106
4-3	π Molecular Orbitals	109
4-4	Energy Levels for BF_3	111
4-5	Equivalence of σ_x and σ_y Orbitals	112
4-6	Ground State of BF_3	114
4-7	Valence Bonds for BF_3	115
4-8	Other Trigonal-Planar Molecules	117

V Tetrahedral Molecules	120
5-1 CH ₄	120
5-2 Ground State of CH ₄	122
5-3 The Tetrahedral Angle	122
5-4 Valence Bonds for CH ₄	125
5-5 Other Tetrahedral Molecules	127
Trigonal-Pyramidal Molecules	
6-1 NH ₃	129
6-2 Overlap in σ_x , σ_y , and σ_z	130
6-3 The Interelectronic Repulsions and H—N—H Bond Angle in NH ₃	
6-4 Bond Angles of Other Trigonal-Pyramidal Molecules	137
6-5 Ground State of NH ₃	138
Angular Triatomic Molecules	141
7-1 H ₂ O	141
7-2 Ground State of H ₂ O	143
7-3 Angular Triatomic Molecules with π Bonding: NO ₂	148
7-4 σ Orbitals	148
7-5 π Orbitals	148
7-6 Ground State of NO ₂	152
Bonding in Organic Molecules	155
8-1 Introduction	155
8-2 C ₂ H ₄	156
8-3 Energy Levels in C ₂ H ₄	159
8-4 Ground State of C ₂ H ₄	159
8-5 Bent-Bond Picture of C ₂ H ₄	160
8-6 Bond Properties of the C=C Group	162
8-7 The Value of β_{cc} in C ₂ H ₄	164
8-8 H ₂ CO	164
8-9 Ground State of H ₂ CO	165

8-10	the $n \rightarrow \pi^*$ Transition Exhibited by the Carbonyl Group	167
8-11	C_2H_2	167
8-12	Ground State of C_2H_2	168
8-13	CH_3CN	168
8-14	C_6H_6	170
8-15	Molecular-Orbital Energies in C_6H_6	171
8-16	Ground State of C_6H_6	173
8-17	Resonance Energy in C_6H_6	173

IX	Bonds Involving d Valence Orbitals	176
9-1	Introduction	176
9-2	The Octahedral Complex $Ti(H_2O)_6^{3+}$	176
9-3	Energy Levels in $Ti(H_2O)_6^{3+}$	179
9-4	Ground State of $Ti(H_2O)_6^{3+}$	181
9-5	The Electronic Spectrum of $Ti(H_2O)_6^{3+}$	183
9-6	Valence-Bond Theory for $Ti(H_2O)_6^{3+}$	184
9-7	Crystal-Field Theory for $Ti(H_2O)_6^{3+}$	186
9-8	Relationship of the General Molecular-Orbital Treatment to the Valence-Bond and Crystal-Field Theories	187
9-9	Types of π Bonding in Metal Complexes	188
9-10	Square-Planar Complexes	189
9-11	Tetrahedral Complexes	194
9-12	The Value of Δ	197
9-13	The Magnetic Properties of Complexes: Weak- and Strong-Field Ligands	200
9-14	The Electronic Spectra of Octahedral Complexes	201

Suggested Reading

Appendix: Atomic Orbital Ionization Energies

Index