

Contents

Preface	v
1 Introduction	1
2 Hückel Theory	8
2.1 The Secular Equations	9
2.2 Matrix Formation	12
2.3 Solution of the Secular Equations	13
A. The Polynomial Method	14
B. Matrix Diagonalization	17
2.4 Charge Densities, Bond Orders and Free Valences	19
2.5 Computer Programs with Listings	22
A. Data Specification	30
B. Computed Results	33
2.6 Problems	38
2.7 References	39
3 Parametric Properties of Hückel Equations	40
3.1 Properties of the Secular Equations	44
3.2 Properties of Polarizability Coefficients	45
3.3 Pairing Properties of Conjugate Solutions	49
3.4 Computer Programs	54
A. Computed Results	55
B. Listings	56
3.5 Problems	56
3.6 References	58
4 Applications of Hückel Theory	59
4.1 Mesomeric Effects in Conjugated Molecules	62
4.2 Variations of α and β	65
A. Changes of Coulomb Integral	67
B. Changes of Resonance Integrals	71
C. Bond "localization"	72
D. Some Areas of Application	73

4.3	Dipole Moments in Conjugated Molecules	77
4.4	Transition Moments in π -Electron Systems	82
4.5	$d_{\pi-p\pi}$ Bonding	90
4.6	Computer Programs	102
	A. Results	110
	B. Listings	112
4.7	Problems	115
4.8	References	119
5	Reactivity Indices in Molecular Orbital Theory	120
5.1	Molecular Orbital Theories of Reactivity	121
	A. The Isolated Molecule Method	123
	B. The Localization Method	124
5.2	Reactivity Indices in Practice	126
5.3	Theoretical Relationships between Reactivity Indices	129
	A. Reactivity Indices in Alternant Hydrocarbons	129
	B. Reactivity Indices in Heteromolecules	132
5.4	Analysis of Models by Computer Methods	135
5.5	Reactivity Indices and Localized π -Complexes	140
5.6	Problems	144
5.7	References	145
6	The Self Consistent Field Method	147
6.1	Solution of SCF Equations	152
6.2	SCF Core and Electron Repulsion Integrals	154
6.3	Properties of SCF Equations	157
	A. Even Alternant Hydrocarbons.	157
	B. Properties of Perturbation Coefficients	158
6.4	Variations of Parameter ω and γ	160
6.5	Applications of SCF-MO Methods	162
	A. Cyclic Polyenes	162
	B. Borazine $B_3N_3H_6$	165
6.6	Note on Programs and Problems	168
6.7	References	169
7	Configuration Interaction and Excited States	170
7.1	The Configuration Interaction Method	171
	A. Alternant Hydrocarbons	174
	B. Heteromolecules	177
7.2	Transition Intensities	180

Contents	xi
7.3 Applications of SCF-CI Methods	182
7.4 Computer Programs	186
A. Results	193
B. Listings	197
7.5 References	206
Subject Index	207