

CONTENTS

1. Colour and Colour Measurement	
1.1 Introduction	1
1.2 What is Colour?	3
1.3 Other Factors Influencing Colour	9
1.4 Colour Vision	10
1.5 The Measurement of Colour	12
1.6 Electronic Absorption Spectroscopy	13
Bibliography	17
2. Quantitative Applications of Molecular Orbital Theory to Electronic Excitation	
2.1 Molecular Orbitals and Light Absorption	18
2.2 The Free Electron Molecular Orbital (FEMO) Method	24
2.3 The Huckel Molecular Orbital (HMO) Method	28
2.4 Some Applications of HMO Theory to Electronic Spectra	35
2.5 Electron Densities and Bond Orders	36
2.6 Alternant and Nonalternat Hydrocarbons	38
2.7 The Pariser-Parr-Pople (PPP) Self Consistent Field Molecular Orbital Method	41
2.8 Configuration Interaction (CI)	47
2.9 More Advanced Molecular Orbital Methods	51
References	53
Bibliography	54
3. Physical Aspects of Light Absorption	
3.1 The light Absorption Process	55
3.2 Energy Conversion I Excited States	57
3.3 Orbital Symmetry and Transition Intensities	59
3.4 Molecular Orbital Theory and the Calculation of Intensities	64
3.5 Polarisation of Absorption Bands	68
3.7 Intermolecular Effects on Absorption Spectra	75
References	80
4. Qualitative Colour-Structure Relationships	
4.1 The Classification of Coloured Organic Molecules	81
4.2 Resonance Theory and Colour	85
4.3 Failures of Resonance Theory	89
4.4 Perturbational Molecular Orbital Theory	92
4.5 Other Empirical Approaches to Substituent Effects	100
4.6 Steric Effects in Electronic Absorption Spectra-General Consideration	104
4.7 Steric Effects in Cyanine-Type Chromogens	109
4.8 Allopolar Isomerism	114

References	115
5 $n \rightarrow \pi^*$ Chromogens	117
5.1 General Characteristics of $n \rightarrow \pi^*$	117
5.2 The Carbonyl Group	121
5.3 The Imino Group	125
5.4 The Azo Group	129
5.5 The Nitroso Group	133
5.6 The Thionitroso Group	135
5.7 The Thiocarbonyl Group	136
References	139
6. Donor-Acceptor Chromogens-I. Simple Acceptors	
6.1 General Characteristics of Donor-Acceptor Chromogens	140
6.2 The Carbonyl Acceptor: Merocyanine-Type Compounds	146
6.3 Solvent Effects in Merocyanine-Type Compounds	153
6.4 Some Merocyanine-Type Chromogens of Technical Interest	158
6.5 The Nitro Acceptor Group	160
6.6 Nitro Analogues of the Merocyanine-Type Chromogens	161
6.7 Donor-Substituted Nitroaromatics-Type Chromogens	161
6.8 Nitrodiphenylamines	166
6.9 Nitrophenylhydrazones	168
6.10 The Cyano Acceptor	169
References	171
7. Donor-Acceptor Chromogens-II. Complex Acceptors	
7.1 Classes of Complex Acceptor Residues	172
7.2 Donor-Substituted Quinones	173
7.3 Donor-Substituted Azo Compounds	180
7.4 Colour and Constitution of the Simple Azo Dyes	181
7.5 Steric Effects in the Monoazo Dyes	186
7.6 Azo-Hydrazone Tautomerism in the Simple Azo Dyes	189
7.7 Protonation Equilibria of Aminoazo Dyes	192
7.8 Metal Complexes of Ortho-Hydroxyazo Dyes	193
7.9 Indigoid Dyes and Related Chromogens	195
7.10 Zwitterionic Chromogens	200
References	202
8. Chromogens Based on Acyclic and Cyclic Polyene Systems	
8.1 General Characteristics	205
8.2 Acyclic Polyenes	208
8.3 Some Coloured Polyene Systems of Technical and Biological Interest	212
8.4 Polycyclic Benzenoid Compounds	215
8.6 Non-Benzenoid Alternant Cyclic Systems-The Annulenes	223

8.7 Non-Benzenoid Alternant Cyclic Systems-The Porphyrins	227
8.8 Nonalternant Polyene Chromogens	233
References	238
9. Cyanine-Type Chromogens\	
9.1 General Characteristics	240
9.2 The Cyanine Dyes	245
9.3 Amino Substituted Di-and Tri-Arylmethane Dyes	250
9.4 The Oxonols, Hydroxyarylmethanes, and Related Chromogens	257
9.5 Heterocyclic Analogues of the Diarylmethane Dyes	262
9.6 Nitro Anions as Cyanine-Type Chromogens	265
References	269
Subject Index	271