

CONTENTS

Chapter 1	An Introduction to the Theory of Light Absorption	1
1.1	Early theories of colour	
1.2	The spectrum	
1.3	The fundamental postulates of quantum mechanics	
1.4	The absorption and emission of light	
1.5	Sources of experimental data	
Chapter 2	Molecular Wave Functions	11
2.1	The separation of electronic and nuclear motions	
2.2	Electron spin	
2.3	Orbitals and Slater determinants	
2.4	Energy calculations	
2.5	Symmetry	
Chapter 3	Valence-bond and Molecular-orbital Theories	30
3.1	Valence-bond theory	
3.2	Free-electron molecular orbitals	
3.3	The LCAO approximation	
3.4	A comparison of valence-bond and molecular-orbital theories	
Chapter 4	The Absorption Spectra of Ethylene and Acetylene	47
4.1	Ethylene	
4.2	Chromophores which are iso-electronic with the ethylenic group	
4.3	Acetylene	
4.4	Conclusions	
Chapter 5	Conjugated Hydrocarbon Chains	67
5.1	Conjugation	
5.2	Linear polyenes	
5.3	Polyacetylenes and cumulenes	
5.4	Polymethine dyes	
5.5	Cyclic polyenes and related compounds	

Chapter 6	Benzenoid Hydrocarbons	91
6.1	The general features of benzenoid spectra	
6.2	Empirical calculations of energy levels	
6.3	Vibrational structure	
6.4	Benzene	
Chapter 7	Weakly Interacting Chromophores	133
7.1	Non-conjugated chromophores	
7.2	Conjugated chromophores with weak electron delocalization	
Chapter 8	Transitions of Non-bonding Electrons	158
8.1	The carbonyl group	
8.2	Dialdehydes, diketones and quinones	
8.3	Acids and amides	
8.4	Sulphur compounds	
8.5	The nitrogen heterocyclics	
8.6	The azo group $-N=N-$	
8.7	Nitrogen-oxygen links	
Chapter 9	The Inductive Effect	189
9.1	Introduction to substituent effects	
9.2	Heteroconjugated molecules	
9.3	The inductive effect of a substituent	
Chapter 10	The Mesomeric Effect	211
10.1	Introduction	
10.2	A weak mesomeric effect	
10.3	A strong mesomeric effect	
Chapter 11	Steric Effects	238
Chapter 12	Non-alternant Hydrocarbons, Hydrocarbon Radicals and Ions	247
12.1	Non-alternant hydrocarbons	
12.2	Hydrocarbon radicals	
12.3	Carbanions and carbonium ions	
Chapter 13	The Spectra of Molecular Complexes	270
Chapter 14	Fluorescence and Phosphorescence	284
14.1	Paths of excitation and emission	
14.2	Spin decoupling	
14.3	Applications of emission spectra	

Appendix 1

The reduction of many-electron integrals to one and two-electron integrals.

Appendix 2

Matrix elements of the Hamiltonian between the lowest states of a molecule having a closed-shell ground state.

Appendix 3

Perturbation theory using a set of non-orthogonal functions.

Appendix 4

The symbols of symmetry groups and their representations.

Appendix 5

A calculation of the 1L_a band energy of naphthalene by the P-method.

Appendix 6

Energy–wavelength conversion table