

Contents

CHAPTER I	SCATTERING BY AN ELECTRON	
	I.1 Introduction	1
	I.2 X-Ray beams	2
	I.3 Polarised X-rays	3
	I.4 Unpolarised X-rays	4
	I.5 Compton effect	5
	I.6 Summary	6
CHAPTER II	DIFFRACTION AS FOURIER TRANSFORMATION	
	II.1 Introduction	7
	II.2 Scattering by an electron density distribution	7
	II.3 Representation of scattered waves	8
	II.4 Properties of the Fourier transform	10
	II.5 Light	13
	II.6 Neutrons and electrons	14
	II.7 Summary	16
CHAPTER III	PRINCIPLES OF STRUCTURE DETERMINATION	
	III.1 Introduction	17
	III.2 Phase problem	17
	III.3 Patterson function	18
	III.4 Solution by deduction	19
	III.5 Trial-and-error solution	24
	III.6 Resolution	24
	III.7 Loss of information at low Q values	27
	III.8 Chirality	28
	III.9 Summary	30

CHAPTER IV	DIFFRACTION GEOMETRY	
	IV.1	Introduction 31
	IV.2	Ewald sphere 31
	IV.3	Q-space 33
	IV.4	Simulation by optical diffraction 37
	IV.5	Summary 39
CHAPTER V	ATOMS AND MOLECULES	
	V.1	Introduction 40
	V.2	Atoms 40
	V.3	Molecules 42
	V.4	Molecules at low resolution 43
	V.5	Anomalous scattering 45
	V.6	Determination of chirality 50
	V.7	Summary 50
CHAPTER VI	IDEAL GASES AND SOLUTIONS	
	VI.1	Introduction 51
	VI.2	Scattered intensity distribution 51
	VI.3	Intensity at low Q values 54
	VI.4	Solutions of macromolecules 54
	VI.5	Deduction of molecular structure 56
	VI.6	Guinier's law 58
	VI.7	Smearing 62
	VI.8	Summary 63
CHAPTER VII	LIQUIDS AND AMORPHOUS SOLIDS	
	VII.1	Introduction 64
	VII.2	Intermolecular interference 65
	VII.3	Appearance of diffraction patterns 70
	VII.4	Determination of the arrangement of molecules 72
	VII.5	Theories of $g(r)$ for liquids 73
	VII.6	Summary 75
CHAPTER VIII	ONE-DIMENSIONAL CRYSTALS	
	VIII. 1	Introduction 76
	VIII. 2	Interference effects 76
	VIII. 3	Formation of the diffraction pattern 80
	VIII. 4	Intensity of the layer lines 85
	VIII. 5	Deduction of electron density 86
	VIII. 6	Bragg's law 87
	VIII. 7	Disorder 87
	VIII. 8	Mosaic spread 89
	VIII. 9	Lorentz correction 90
	VIII.10	Summary 93

CHAPTER IX	HELICES AND LIQUID CRYSTALS	
	IX.1 Introduction	94
	IX.2 Continuous helix	94
	IX.3 Discontinuous helix	102
	IX.4 Molecular helix	107
	IX.5 Nematic organisation	110
	IX.6 Smectic organisation	115
	IX.7 Summary	117
CHAPTER X	THREE-DIMENSIONAL CRYSTALS	
	X.1 Introduction	119
	X.2 Intensity distribution	119
	X.3 Diffraction geometry	125
	X.4 Determination of crystal structures	129
	X.5 Symmetry	131
	X.6 Summary	133
CHAPTER XI	CRYSTALLINE POWDERS AND CRYSTALLINE FIBRES	
	XI.1 Introduction	134
	XI.2 Powder method	134
	XI.3 Crystalline fibres	136
	XI.4 Interpretation of crystalline fibre patterns	139
	XI.5 Summary	141
CHAPTER XII	RELATIONSHIP TO MICROSCOPY	
	XII.1 Introduction	142
	XII.2 Fourier transformation and microscopy	142
	XII.3 Atomic resolution	145
	XII.4 Electron microscopy and diffraction	147
	XII.5 Summary	151
BIBLIOGRAPHY		152
INDEX		157