Preface and Acknowledgments xi

SECTION 1 Symmetry and Space Groups

Chapter 1 Introduction

3 (12)

Chapter 2 Point Symmetry Operations

15 (12)

Chapter 3 Point Groups

27 (16)

Chapter 4 Periodicity

43 (12)

Chapter 5 Travel Symmetry Operations

55 (12)

Chapter 6 Two-dimensional Lattices

67 (12)

Chapter 7 Three-dimensional Lattices

79 (8)

Chapter 8 Two-dimensional Plane Groups

87 (12)

Chapter 9 Equivalent Positions

99 (12)

Chapter 10 Three-dimensional Space Groups, Part 1

111 (10)

Chapter 11 Three-dimensional Space Groups, Part 2

121 (12)

Chapter 12 Three-dimensional Space Groups, Part 3

133 (12)

SECTION 2 X-rays and Diffraction

Chapter 13 Generation of X-rays

145 (12)

Chapter 14 Diffractometers and Data Collection

157 (10)

Chapter 15 Data Reduction

167 (12)

Chapter 16 Scattering from a Single Electron

179 (10)

Chapter 17 Scattering from Atoms

189 (10)

Chapter 18 Diffraction from One-dimensional Arrays

199 (8)

Chapter 19 Diffraction from Two- and Three-dimensional Arrays

207 (12)

Chapter 20 Reciprocal Space and Reflection Indices

219 (6)

Chapter 21 Bragg's Law, Scattering Planes, and d-Spacings

225 (10)

Chapter 22 The Limiting Sphere, Resolution, and Indexing

235 (12)

Chapter 23 Structure Factors and Argand Diagrams

247 (8)

Chapter 24 Phases, Friedel's Law, and Laue Classes

255 (10)

Chapter 25 Centrosymmetry and Chirality

265 (12)

Chapter 26 Reflection Conditions

277 (12)

Chapter 27 Determining the Space Group of a Crystal

289 (10)

SECTION 3 Solving and Refining Crystal Structures

Chapter 28 Fourier Transforms in Crystallography

299 (10)

Chapter 29 Trial-and-error Methods

309 (10)

Chapter 30 Charge Flipping

319 (8)

Chapter 31 The Patterson Method

327 (8)

Chapter 32 The Heavy Atom Approximation

335 (14)

Chapter 33 Protein Crystal Structures

349 (12)

Chapter 34 Direct Methods, Part 1

361 (10)

Chapter 35 Direct Methods, Part 2

371 (12)

Chapter 36 Modeling the Electron Density

383 (12)

Chapter 37 Refining Crystal Structures

395 (12)

Chapter 38 Twinning

407 (10)

Chapter 39 Examples of Twinned Crystals

417 (10)

Chapter 40 Mistakes and Pitfalls

427 (12)

Chapter 41 Powder X-ray Diffraction

439 (12)

Chapter 42 Electron and Neutron Diffraction

451 (6)

Appendix A Vector Tutorial 457 (6)

Appendix B Complex Number Tutorial 463 (4)

Appendix C The Ewald Sphere 467 (6)

Appendix D Atomic Form Factors 473 (6)

Appendix E The Patterson Function 479 (4)

Appendix F In-class Demonstration of Diffraction 483 (4)

Bibliography 487 (4)

Index 491