International Tables for Crystallography, Volume B: International Tables for Crystallography, Reciprocal Space (IUCr Series. International Tables of Crystallography)

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Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research. After an introductory chapter, Part 1 presents the reader with an account of structure-factor formalisms, an extensive treatment of the theory, algorithms and crystallographic applications of Fourier methods, and fundamental as well as advanced treatments of symmetry in reciprocal space. In Part 2, these general accounts are followed by detailed expositions of crystallographic statistics, the theory of direct methods, Patterson techniques, isomorphous replacement and anomalous scattering, and treatments of the role of electron microscopy and diffraction in crystal structure determination, including applications of direct methods to electron crystallography. Part 3 deals with applications of reciprocal space to molecular geometry and `best'-plane calculations, and contains a treatment of the principles of molecular graphics and modelling and their applications. A convergence-acceleration method of importance in the computation of approximate lattice sums is presented and the part concludes with a discussion of the Ewald method. Part 4 contains treatments of various diffuse-scattering phenomena arising from crystal dynamics, disorder and low dimensionality (liquid crystals), and an exposition of the underlying theories and/or experimental evidence. Polymer crystallography and reciprocal-space images of aperiodic crystals are also treated. Part 5 of the volume contains introductory treatments of the theory of the interaction of radiation with matter (dynamical theory) as applied to X-ray, electron and neutron diffraction techniques.

The simplified trigonometric expressions for the structure factors in the 230 three-dimensional space groups, which appeared in Volume I of International Tables for X-ray Crystallography, are now given in Appendix 1.4.3 to Chapter 1.4 of this volume.

Volume B is a vital addition to the library of scientists engaged in crystal structure determination, crystallographic computing, crystal physics and other fields of crystallographic research. Graduate students specializing in crystallography will find much material suitable for self-study and a rich source of references to the relevant literature.

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