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Crystallographic Computing 6

A Window on Modern
Crystallography

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and Kálmán Simon

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Crystallographic Computing 6 A Window On Modern Crystallography

Philip Coppens



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crystallography The main aim in the book is to show how computer simulation of a model crystal provides a general method by which diffuse scattering of all kinds and from all types of materials can be interpreted and analysed Part I of the book gives a description of the experimental methods used to obtain diffuse scattering data Part II describes a number of simple stochastic models of disorder which allows various concepts to be established and enables simple examples to be generated to illustrate key principles Part III describes example studies of a wide variety of real materials These examples not only document the development of computer simulation methods for investigating and analysing disorder problems but also provide a resource for helping future researchers recognise the kinds of effects which can occur and for pointing the way to tackling new problems which are encountered

Macromolecular Crystallography Charles W. Carter, Robert M. Sweet, 1997 Crystallographic Computing, 1993 Correlations, Transformations, and Interactions of Organic Crystal Structures Derry Wynn Jones, Andrzej Katrusiak, 1994 Structural crystallographic analysis can reveal the stereochemistry and detailed molecular arrangement of chemical species and series of compounds in the solid state Based on the Eighth International Symposium on Organic Crystal Chemistry this volume provides accessible overviews of topics in the forefront of contemporary organic molecule crystallography Topics include special techniques for collection and treatment of diffraction data crystalline state reactions structure correlation from the database and structure activity relations as well as molecular crystal conformation packing and hydrogen bonding Students and researchers in crystallography and organic chemistry will want to own a copy of this book

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