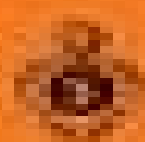


Crystallographic Statistics in Chemical Physics



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International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Each of the volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials Emphasis is given to symmetry diffraction methods and techniques of crystal structure determination and the physical and chemical properties of crystals The data are accompanied by discussions of theory practical explanations and examples all of which are useful for teaching Volume G deals with methods and tools for organizing archiving and retrieving crystallographic data The volume describes the Crystallographic Information File CIF the standard data exchange and archival file format used throughout crystallography The volume is divided into five parts Part 1 An introduction to the development of CIF Part 2 Details concepts and specifications of the files and languages Part 3 Discusses general considerations when defining a CIF data item and the classification and use of data Part 4 Defines all the data names for the core and other dictionaries Part 5 Describes CIF applications including general advice and considerations for programmers The accompanying software includes the CIF dictionaries in machine readable form and a collection of libraries and utility programs Volume G is an essential guide for programmers and data managers handling crystal structure information and provides in depth information vital for recording or using single crystal or powder diffraction data in small molecule inorganic and biological macromolecular structure science More information on the series can be found at <http://it.iucr.org> *World Directory of Crystallographers* Allan L. Bednowitz, Armin P. Segmüller, 2013-04-17 A brief historical account of the background leading to the publication of the first four editions of the World Directory of Crystallographers was presented by G Boom in his preface to the Fourth Edition published late in 1971 That edition was produced by traditional typesetting methods from compilations of biographical data prepared by national Sub Editors The major effort required to produce a directory by manual methods provided the impetus to use computer techniques for the Fifth Edition The account of the production of the first computer assisted Directory was described by S C Abrahams in the preface of the Fifth Edition Computer composition which required a machine readable data base offered several major advantages The choice of typeface and range of characters was flexible Corrections and additions to the data base were rapid and once established it was hoped updating for future editions would be simple and inexpensive The data base was put to other Union uses such as preparation of mailing labels and formulation of lists of crystallographers with specified common fields of interest The Fifth Edition of the World Directory of

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materials science Edward Prince, 2013-07-01 In the course of 30 years as a practicing crystallographer I have frequently been faced with the necessity of finding out a little bit about some general branch of mathematics with which I was previously unfamiliar Under these circumstances I have usually followed the common practice of seeking out some colleague who would be expected to have a thorough knowledge of the subject I would then find myself faced either with an involved lecture in which the colleague would attempt to distill a lifetime of experience into a form that was comprehensible to a novice with a very different background or with a book about the subject written by a specialist that contained far more information than I really wanted to know I would have to separate the few kernels of useful material from a large volume of what would probably be wheat to someone else but was chaff to me In the course of that time I have acquired a collection of books to which I frequently refer Most of these have a small number of thoroughly dog eared pages along with many that have scarcely been opened During the same period I have been privileged to associate and collaborate with a number of materials scientists who were not trained as crystallographers but whose interests required them to understand particular details of some structural problem Crystallographic Databases, 1987 *Physical and chemical* Alfred Edwin Howard Tutton, 1922 **Science Abstracts**, 1904 *Subject Guide to Books in Print*, 1991 Introduction to Crystallographic Statistics Uri Shmueli, George Herbert Weiss, 1995 Modern structural applications of crystallography make extensive use of statistical methods in particular the probability density function pdf of the magnitude of the structure factor Similarly direct methods of phase determination have been responsible for much of the success of crystallography methods based on properties of joint pdfs This monograph from two authorities in the field of structure factor statistics presents a survey of techniques and theories in this field of research in a self contained and consistent way with an emphasis on the probabilistic principles involved **International Workshop on Evaluation of Single-Crystal Diffraction Data from 2-D Position-Sensitive Detectors**, 1986

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