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merican Crystallographic Association

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Solution Of The Phase Problem The Centro

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Crystal Structure Determination H. Hauptman, 2013-04-17 The central theme of this monograph is that the cosine seminvariants are the key to crystal structures The cosine seminvariants are the cosines of those linear combinations of the phases the so called structure seminvariants whose values for a given functional form for the geometric structure factor are uniquely determined by the crystal structure alone and are therefore independent of the choice of permissible origin It follows that the cosine seminvariants themselves are uniquely determined in general by the observed magnitudes of the normalized structure factors The values of the cosine seminvariants in turn lead unambiguously to the values of the individual phases and thus to the crystal structure by means of the E map Fourier synthesis It is this property of the cosine seminvariants that they serve to link the observed magnitudes with the desired phases of the normalized structure factors which accounts for their importance and explains the emphasis which is here placed on their role **Theory and Practice**

of Direct Methods in Crystallography M. F. C. Ladd, R. A. Palmer, 2012-12-06 Direct methods of crystal structure determination are usually associated with techniques in which phases for a set of structure factors are determined from the corresponding experimental amplitudes by probabilistic calculations It is thus implied that such ab initio phase calculations do not require a knowledge of atomic positions and this basis distinguishes direct methods from other techniques for structure determination An acceptably wider interpretation of the term direct methods leads to other important applications involving inter alia the use of heavy atoms resolution limited phase data for large molecules rotation functions and Fourier series These topics are discussed in the later chapters of this book Although some earlier theoretical investigations were made by Harker and Kaspar direct methods may be considered to have begun around the year 1950 Important landmarks in the development of the subject include the book by Hauptmann and Karle *The Centrosymmetric Crystal* 1953 the definitive paper by Karle and Karle in *Acta Crystallographica* 1966 and the recent 1978 sophisticated program package MULTAN 78 produced mainly by Germain Main and Woolfson Woolfson's book *Direct Methods in Crystallography* was published in 1961 but because of the rapid progress in direct methods much of it soon became outmoded It is interesting to note that direct methods nearly came into being many years earlier Certainly the E2 relationship was used implicitly by Lonsdale in 1928 in determining the crystal structure of hexamethylbenzene *Determination of Organic Structures by Physical Methods V3*

F.C. Nachod, 2012-12-02 *Determination of Organic Structures by Physical Methods Volume 3* is a seven chapter text that describes the refinements of some established physical methods for organic structure determination Each chapter of this book examines specific physical method including photoelectron spectroscopy X ray diffraction optical rotary dispersion circular dichroism mass spectrometry and electron spin resonance and NMR spectroscopies The historical developments instrumentation and applications to organic chemistry of these methods are discussed This work will be of value to organic and analytical chemists and researchers **Handbook of Solid State Chemistry, 6 Volume Set** Richard

Dronskowski, Shinichi Kikkawa, Andreas Stein, 2017-10-23 This most comprehensive and unrivaled compendium in the field provides an up to date account of the chemistry of solids nanoparticles and hybrid materials Following a valuable introductory chapter reviewing important synthesis techniques the handbook presents a series of contributions by about 150 international leading experts the Who's Who of solid state science Clearly structured in six volumes it collates the knowledge available on solid state chemistry starting from the synthesis and modern methods of structure determination Understanding and measuring the physical properties of bulk solids and the theoretical basis of modern computational treatments of solids are given ample space as are such modern trends as nanoparticles surface properties and heterogeneous catalysis Emphasis is placed throughout not only on the design and structure of solids but also on practical applications of these novel materials in real chemical situations *Computing Methods and the Phase Problem in X-ray Crystal Analysis* Ray Pepinsky, 1952

Advances in Computers, 1964-01-01 The survey articles included in Volume 5 have been selected with two aims in mind to arrive at a balanced sampling of the computer field and to emphasize the subjects of most active current interest Articles cover topics such as the role of computers in delivering election results the state of computer development in the Soviet Union and its neighbors artificial intelligence and applications of computers to the design of optical instruments to nuclear reactor design and to the determination of the structure of crystals or molecules from X ray diffraction patterns **Acta Crystallographica**, 1959-07 *The Statistical Approach to X-ray Structure Analysis* Vladimir Vand, Ray Pepinsky, 1953

Methods of Experimental Physics, 1959 *Seminar on Experimental Molecular Structure II*, 1962 **Proceedings of the IBM Scientific Computing Symposium on Combinatorial Problems**, 1966 Automatic Control 1990 Ü

Jaaksoo, 2014-05-23 This volume provides a general overview on the state of the art and future developments in automation and control The application of systems and control in all areas is covered from the social and cultural effects of control to control in mineral and metal processing This volume will be an invaluable source of information to all those interested in the areas of automation and control **Determination of the Absolute Configuration of Optically Active Compounds by Means of X-rays** Antonius Franciscus Peerdeman, 1955 Frontiers of Chemistry Keith J. Laidler, 2013-10-22 Frontiers of Chemistry reviews the plenary and keynote lectures presented in the 28th International Union of Pure and Applied Chemistry IUPAC Congress The book discusses the future development and applications of chemistry The text is divided into two main parts where the first part covers the plenary lectures and the second part covers the keynote lectures Part 2 is organized into sections according to contents such as the role of chemistry in the solution of energy problems the study of the environment and the beneficiation of resources The book will be of great interest to chemists since it tackles topics that are significant in the advancement of the field of chemistry **Crystallographic Computing** F. R. Ahmed, S. R. Hall, C. P. Huber, 1970

Biophysical Chemistry of Proteins Engelbert Buxbaum, 2025-07-10 This textbook designed for all scientists interested in protein research provides a thorough overview of laboratory methods for the biophysical chemistry of proteins This new

edition completely restructured and expanded for ease of learning includes sections on analytical techniques working with proteins protein size and shape protein structure enzyme kinetics industry enzymology and a new section on special statistics

Energy Research Abstracts ,1989 *Technical Information Pilot* ,1952 **10th International Symposium on Process Systems Engineering** Rita Maria de Brito Alves,Cláudio Augusto Oller do Nascimento,Evaristo Chalbaud Biscaia (Jr),2009 The 10th International Symposium on Process Systems Engineering PSE 09 will be held in Salvador Bahia Brazil on August 16 20 2009 The special focus of PSE 2009 is Sustainability Energy and Engineering PSE 2009 is the tenth in the triennial series of international symposia on process systems engineering initiated in 1982 The meeting is brings together the worldwide PSE community of researchers and practitioners who are involved in the creation and application of computing based methodologies for planning design operation control and maintenance of chemical and petrochemical process industries PSE 09 will look at how the PSE methods and tools can support sustainable resource systems and emerging technologies in the areas of green engineering environmentally conscious design of industrial processes PSE methods and tools support sustainable resource systems emerging technologies in the areas of green engineering environmentally conscious design of industrial processes *Annales Societatis Chimicae Polonorum* ,1978

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