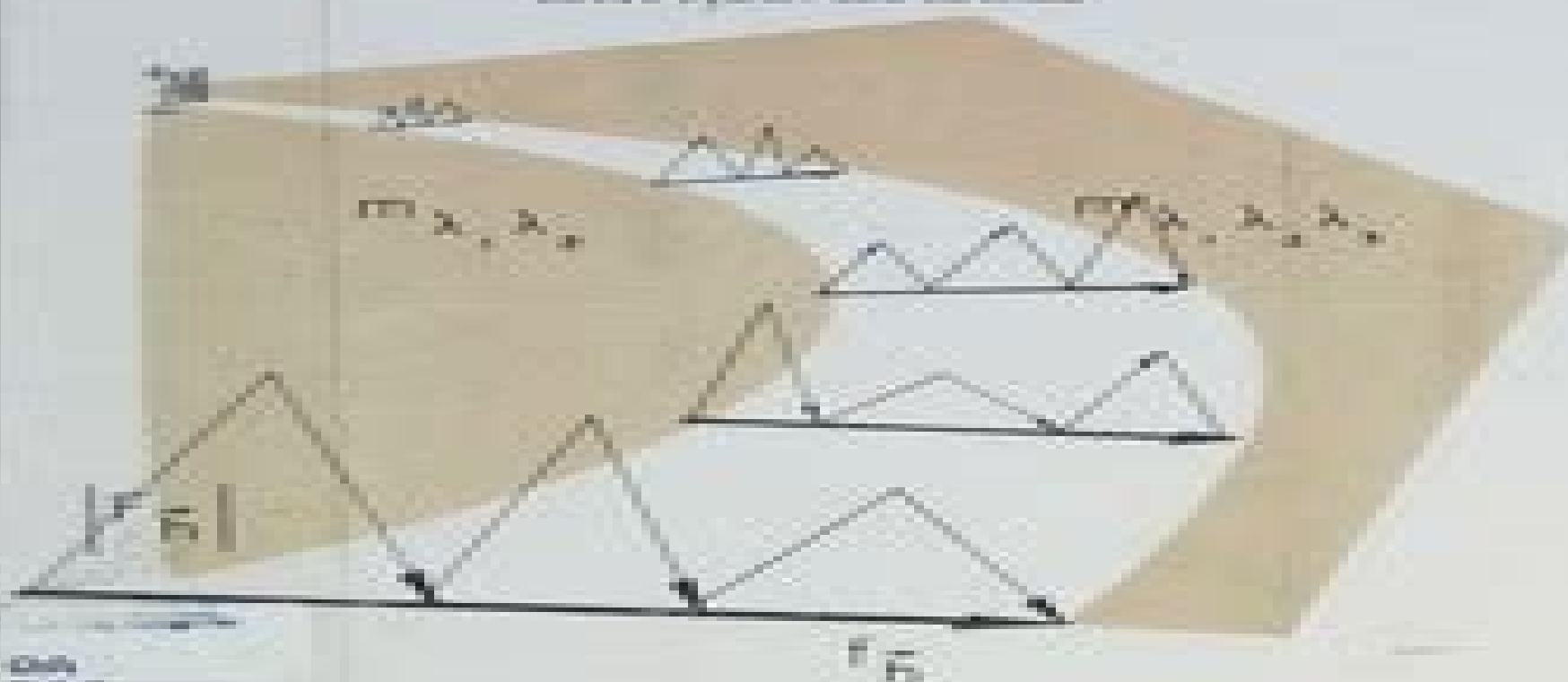


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Crystal Structure Determination H. Hauptman, 2013-04-17 The central theme of this monograph is that the cosine seminvariants are the key to crystal structures The cosine seminvariants are the cosines of those linear combinations of the phases the so 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

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Symposium on Combinatorial Problems, 1966 **10th International Symposium on Process Systems Engineering - PSE2009** Rita Maria de Brito Alves, Claudio Augusto Oller do Nascimento, Evaristo Chalbaud Biscaia, 2009-08-05 This book contains the proceedings of the 10th of a series of international symposia on process systems engineering PSE initiated in 1982 The special focus of PSE09 is how PSE methods can support sustainable resource systems and emerging technologies in the areas of green engineering Contains fully searchable CD of all printed contributions Focus on sustainable green engineering 9 Plenary papers 21 Keynote lectures by leading experts in the field Acta Crystallographica, 1959-07

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Numerical Simulation of Oscillatory Convection in Low-Pr Fluids Bernard Roux, 2013-03-08 For the last ten years there has been an ever increasing awareness that fluid motion and transport processes influenced by buoyancy are of interest in many fields of science and technology In particular a lot of research has been devoted to the oscillatory behaviour of metallic melts low Pr fluids due to the very crucial impact of such flow oscillations on the quality of growing crystals semi conductors or metallic alloys for advanced technology applications Test cases on the 2D oscillatory convection in differentially heated cavities containing low Pr fluids have been defined by the organizing committee and proposed to the community in 1987 The GAMM Workshop was attended by 55 scientists from 12 countries in Oct 1988 in Marseille France Twenty eight groups contributed to the mandatory cases coming from France 12 other European countries 7 and other countries USA Japan and Australia 9 Several groups also presented solutions of various related problems such as accurate determination of the threshold for the onset of oscillations thermocapillary effect in open cavities and 3D simulations Period doubling quasi periodic behaviour reverse transition and hysteresis loops have been reported for high Grashof numbers in closed cavities The workshop was also open to complementary contributions 5 from experiments and theory stability and bifurcation analysis The book contains details about the various methods employed and the specific results obtained by each

contributor *Synthetic Procedures in Nucleic Acid Chemistry: Physical and physicochemical aids in characterization and in determination of structure* W. Werner Zorbach, R. Stuart Tipson, 1968 Band 2

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