

Computing Methods in Crystallography

Edited by **J.S.Rollett**
Computing Laboratory,
University of Oxford

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SOURCE PROGRAM, PUSH START
000000 C      CRYSTALLOGRAPHIC PROGRAM
000000 C      RECIPROCAL UNIT CELL FROM
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000000 40  DIMENSION A(3), COSA(6), SIN(6)
000000      READ 1, A(1), A(2), A(3), COSA(1), COSA(2), COSA(3)
000000 1  FORMAT (6F10.6)
000000      PRINT 2
000000 2  FORM T (28H A = , B = , C = , COSA = , COSB = , COSC = )
000000      PRINT 1, A(1), A(2), A(3), COSA(1), COSA(2), COSA(3)
000000      DO 10 J = 1, 3
000000          SINAJ(J) = SQRT(1. - COSAJ(J)**2)
000000          COSAJ(J+3) = COSAJ(J)
000000 10  SINAJ(J+3) = SINAJ(J)
000000          DO 20 J = 1, 3
000000              COSAS(J) = (COSA(J+1)*COSA(J+2) - COSAJ(J))
000000              SINAS(J) = SQRT(1. - COSAS(J)**2)
000000 20  SINAS(J+3) = SINAS(J)
000000          DO 30 J = 1, 3
000000              AS(J) = 1./[A(J)*SINAJ(J+1)*SINAS(J+2)]
000000          PRINT 3
000000 3  FORMAT (35H A* = , B* = , C* = , COSA* = , COSB* = , COSC* = )
000000          PRINT 1, AS(1), AS(2), AS(3), COSAS(1), COSAS(2), COSAS(3)
000000          GO TO 40
000000      END
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000000 SW 1 OFF TO IGNORE SUBROUTINES, PUSH START
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000000 PROCESSING COMPLETE
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000000 SUBROUTINES - PUSH START

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Computing Methods In Crystallography

CH Cherryholmes



Computing Methods In Crystallography:

Computing Methods in Crystallography J. S. Rollett, 2016-06-06 Computing Methods in Crystallography is a collection of lectures delivered at a Summer School held in Oxford in August 1962 The book presents the underlying mathematics and computing methods in crystallography The text covers topics on the algebra required for the fundamental operations of transformation of coordinates interpolation approximation of trigonometric and exponential functions solution of linear equations and derivation of latent roots and vectors methods for calculation of structure factors least squares adjustment and Fourier series evaluation the theory and practice of intensity scaling and symmetry determination and methods of direct phase determination Crystallographers physicists and students in allied fields will find the book very useful International Tables for Crystallography, Volume B Uri Shmueli, 2008-08-27 International Tables for Crystallography are no longer available for purchase from Springer For further information please contact Wiley Inc follow the link on the right hand side of this page 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 COMPUTING METHODS IN CRYSTALLOGRAPHY- MEETING- PAPERS. , *Computing Methods in Crystallography. Edited by J.S. Rollett. [By Various Authors.].* John Sydney

ROLLETT,1965 **Computing Methods in Crystallography** Tosio Sakurai,Julio Zukerman Schpector,1979 Mathematics of transformation Algebra of linear transformation Transformation of the crystal lattice Symmetry operations Fourier transformation Practical procedures in crystallographic computing Basic considerations Data reduction Structure factor and least squares Fourier synthesis Molecular model building *Current Methods and Optimization Algorithms for the Refinement of X-Ray Crystal Structures* J Uria,1999-08-19 *Structure Determination by X-Ray Crystallography* Marcus Frederick Charles Ladd,Rex A. Palmer,2003-09-30 This book is an account of crystal symmetry and optical and e ray diffraction techniques for examining single crystals It includes the solution of crystal structures by the current methods worked examples of crystal structure determination problems and solutions for each chapter *International Tables for Crystallography, Volume B* U. Shmueli,2008-08-25 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research This volume 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 New to this edition A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals Three new sections on electron diffraction and electron microscopy in structure determination describing point group and space group determination by convergent beam electron diffraction three dimensional reconstruction and single particle reconstruction Substantial revisions to the chapters on space group representations in reciprocal space direct methods Patterson and molecular replacement techniques and disorder diffuse scattering More information on the series can be found at <http://it.iucr.org> **Structure Determination by X-ray Crystallography** Mark F.C. Ladd,Rex A. Palmer,2003-09-30 I was highly flattered when I was asked by Mark Ladd and Rex Palmer if I would write the Foreword to this Fourth Edition of their book Ladd Palmer is such a well known and classic book on the subject of crystal structure determination one of the standards in the field I did feel daunted by the prospect and wondered if I could do justice to it The determination of crystal structures by X ray crystallography has come a long way since the 1912 discoveries of von Laue and the Braggs In the intervening years great advances have been made so that today it is almost taken for granted that crystal structures can be determined in which hundreds if not thousands of separate atomic positions can be found with apparent ease In the early years the structures of relatively simple materials such as the alkali halides were often argued over and even disputed whereas today we routinely see published structures of most complex molecular crystals including the structures of viruses and proteins *Graphical and Tabular Methods in Crystallography* Thomas Vipond Barker,1922 *Encyclopedia of Computer Science and Technology* Jack Belzer,Albert G. Holzman,Allen Kent,1977-02-01 This comprehensive reference work provides immediate fingertip access to state of the art technology in nearly 700 self contained articles written by over 900

international authorities Each article in the Encyclopedia features current developments and trends in computers software vendors and applications extensive bibliographies of leading figures in the field such as Samuel Alexander John von Neumann and Norbert Wiener and in depth analysis of future directions

International Tables for Crystallography: Reciprocal space ,1984 **Methods and Applications in Crystallographic Computing** Sydney R. Hall,Tamaichi Ashida,1984

Thirty five international authorities offer comprehensive review of current computing techniques in crystal structure analysis The volume contains sections on data measurement and processing solution techniques refinement techniques accurate electron density analysis computer software and hardware data base techniques and computer graphics There are also contributions on powder methods and electron diffraction and microscopy

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