



Crystallographic Computing 3: Data Collection, Structure Determination, Proteins, and Databases

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Raffaella Di Napoli

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Crystallographic Computing 3 International Summer School on Crystallographic Computing, 1985 *Crystallographic Computing 3* G. M. Sheldrick, C. Krüger, R. Goddard, 1985 Papers presented at the International Summer School on Crystallographic Computing M hlein August 1984 *Crystal Structure Analysis for Chemists and Biologists* Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, 1996-12-17 The fields of structural chemistry and biochemistry have blossomed in the last seventy years since X ray diffraction was discovered in 1912 Dorothy Hodgkin who obtained a Nobel Prize in 1965 for her X ray diffraction work wrote a great advantage of X ray analysis as a method of chemical structure analysis is its power to show some totally unexpected and surprising structure with at the same time complete certainty The results of all X ray diffraction studies are used by chemists and buiochemists but these scientists need to be able to appreciate the significance and extent to which these results may be used A number of books written for practicing crystallographers cover the theory and applications of X ray diffraction but few are of real practical use to non specialists In *Crystal Structure Analysis for Biologists and Chemists* the general principles of crystal structure are presented in a highly readable way The book of Glusker who is internationally renowned provides good coverage of theory including data and understanding their significance Current Methods and Optimization Algorithms for the Refinement of X-Ray Crystal Structures J Uria, 1999-08-19 *Direct Methods for Solving Macromolecular Structures* S. Fortier, 2013-06-29 This book of the proceedings of the 1997 NATO Advanced Study Institute ASI on Direct Methods for Solving Macromolecular Structures was assembled from the lecturers contributions and represents a comprehensive and in depth overview of crystallographic structure determination methods for macromolecules While having a focus based on the direct methods the Institute adopted an inclusive and broad perspective Thus both direct and experimental phasing techniques are presented in this book highlighting their complementarities and synergies As weil methodologies spanning the full crystallographic image reconstruction process from low resolution envelope definition to high resolution atomic refinement are discussed The first part of the book introduces the array of tools currently used in structure determination whether originating from a mathematical computational or experimental framework This section of the book displays the variety and ingenuity of old and new phasing approaches developed to solve increasingly complex structures Some of the contributions focus on recent developments and or implementations that have given older approaches a new life A case in point is the re implementation of Buerger s superposition approach which is now solving protein structures Another beautiful example is found in the introduction to the traditional multiple isomorphous replacement approach where new techniques such as site directed mutagenesis and the use of inert gases in the preparation of heavy atom derivatives are described Equally impressive are the presentations of newer approaches which take advantage of advances on the experimental front e g *Reviews in Computational Chemistry, Volume 17* Kenny B. Lipkowitz, Donald B. Boyd, 2003-04-24 Computational chemistry is

increasingly used in most areas of molecular science including organic inorganic medicinal biological physical and analytical chemistry Researchers in these fields who do molecular modelling need to understand and stay current with recent developments This volume like those prior to it features chapters by experts in various fields of computational chemistry Two chapters focus on molecular docking one of which relates to drug discovery and cheminformatics and the other to proteomics In addition this volume contains tutorials on spin orbit coupling and cellular automata modeling as well as an extensive bibliography of computational chemistry books FROM REVIEWS OF THE SERIES Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry JOURNAL OF MOLECULAR GRAPHICS AND MODELLING One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry The basic philosophy of the editors seems to be to help the authors produce chapters that are complete accurate clear and accessible to experimentalists in particular and other nonspecialists in general JOURNAL OF THE AMERICAN CHEMICAL SOCIETY *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> *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 **Journal of the Chinese Chemical Society ...** Chinese Chemical Society, 2004 Index of Conference Proceedings Received British Library. Document Supply Centre, 1986

Chemometrics in Environmental Chemistry - Statistical Methods Jürgen Einax, 2013-04-17 Pattern recognition and other chemometrical techniques are important tools in interpreting environmental data This volume presents authoritatively state of the art procedures for measuring and handling environmental data The chapters are written by leading experts

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