

Experimental phasing opportunities for macromolecular crystallography at very long wavelengths

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Despite recent advances in cryo-electron microscopy and artificial intelligence-based model predictions, a significant fraction of structure determinations by macromolecular crystallography still requires experimental phasing, usually by means of single-wavelength anomalous diffraction (SAD) techniques. Most synchrotron beamlines provide highly brilliant beams of X-rays of between 0.7 and 2 Å wavelength. Use of longer wavelengths to access the absorption edges of biologically important lighter atoms such as calcium, potassium, chlorine, sulfur and phosphorus for native-SAD phasing is attractive but technically highly challenging. The long-wavelength beamline I23 at Diamond Light Source overcomes these limitations and extends the accessible wavelength range to $\lambda = 5.9$ Å. Here we report 22 macromolecular structures solved in this extended wavelength range, using anomalous scattering from a range of elements which demonstrate the routine feasibility of lighter atom phasing. We suggest that, in light of its advantages, long-wavelength crystallography is a compelling option for experimental phasing.

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Macromolecular Crystallography

**Randy Read, Alexandre G.
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Sanderson, Jane V. Skelly, 2007-08-23 Macromolecular crystallography is the study of macromolecules using X ray crystallographic techniques to determine their molecular structure This title synthesises contributions from a team of internationally recognized leaders offering chapters on conventional and high throughput methods **Macromolecular Crystallography, Part D** Charles W. Carter Jr., Charles W. Carter, Robert M. Sweet, 2003-12-10 Accurate molecular structures is vital for rational drug design and for structure based functional studies directed toward the development of effective therapeutic agents and drugs Crystallography can reliably predict structure both in terms of folding and atomic details of bonding Phases Map interpretation and refinement Analysis and software **Macromolecular Crystallography**

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map improvements interpretation of electron density maps automatic structure determination and the dissection of ultra high resolution structures c Book News Inc *Advancing Methods for Biomolecular Crystallography* Randy Read,Alexandre G. Urzhumtsev,Vladimir Y. Lunin,2013-04-03 This work presents a snapshot of the state of the art of modern biomolecular crystallography from crystallisation through structure determination and even interactive presentation on the web Methods driving the latest automated structure determination pipelines are explained as well as how to deal with problems such as crystal pathologies that still demand expert analysis These methods are illustrated through their application to problems of great biological interest such as the molecular machinery underlying the complement pathway the mechanism of action of monoamine oxidase inhibitors and the structure of the eukaryotic ribosome Complementary approaches such as neutron diffraction small angle X ray scattering coherent diffraction and computational modelling are also explored *Biomolecular Crystallography* Bernhard Rupp,2009-10-20 Synthesizing over thirty years of advances into a comprehensive textbook Biomolecular Crystallography describes the fundamentals practices and applications of protein crystallography Illustrated in full color by the author the text describes mathematical and physical concepts in accessible and accurate language Biomolecular Crystallography will be a valuable resource for advanced undergraduate and graduate students and practitioners in structural biology crystallography and structural bioinformatics **Macromolecular Crystallography Protocols** Sylvie Doublié,2007 In the decade since publication of the first edition of Crystallographic Methods and Protocols the field has seen several major developments that have both accelerated the pace of structure determination and made crystallography accessible to a broader range of investigators Volume I Preparation and Crystallization of Macromolecules is dedicated to the crystallization and ways to increase the odds of obtaining crystals in macromolecules while Volume 2 Structure Determination covers both computational methods for characterizing crystals and solving structures

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result of breakthroughs in synthesis and characterization that have taken place over the last few years the book provides the first reference with a focus on these exciting novel nanomaterials explaining their formation and how and why they play an important role in the future of molecular electronics catalysis sensing biological imaging and medical diagnosis and therapy Surveys the fundamental concepts and potential applications of atomically precise metal clusters protected by organic ligands Provides well organized tutorial style chapters that are ideal for teaching and self study In depth descriptions by top scientists in the field Presents the state of the art of protected metal clusters and their future prospects *Current Methods and Optimization Algorithms for the Refinement of X-Ray Crystal Structures* J Uria,1999-08-19 **21st Century**

Challenges in Chemical Crystallography I D. Michael P. Mingos,Paul R. Raithby,2021-01-20 This volume summarises recent developments and possible future directions for small molecule X ray crystallography It reviews specific areas of crystallography which are rapidly developing and places them in a historical context The interdisciplinary nature of the technique is emphasised throughout It introduces and describes the chemical crystallographic and synchrotron facilities which have been at the cutting edge of the subject in recent decades The introduction of new computer based algorithms has proved to be very influential and stimulated and accelerated the growth of new areas of science The challenges which will arise from the acquisition of ever larger databases are considered and the potential impact of artificial intelligence techniques stressed Recent advances in the refinement and analysis of X ray crystal structures are highlighted In addition the recent developments in time resolved single crystal X ray crystallography are discussed Recent years have demonstrated how this technique has provided important mechanistic information on solid state reactions and complements information from traditional spectroscopic measurements The volume highlights how the prospect of being able to routinely watch chemical processes as they occur provides an exciting possibility for the future Recent advances in X ray sources and detectors that have also contributed to the possibility of dynamic single crystal X ray diffraction methods are presented The coupling of crystallography and quantum chemical calculations provides detailed information about electron distributions in crystals and has resulted in a more detailed understanding of chemical bonding The volume will be of interest to chemists and crystallographers with an interest in the synthesis characterisation and physical and catalytic properties of solid state materials Postgraduate students entering the field will benefit from a historical introduction to the subject and a description of those techniques which are currently used Since X ray crystallography is used so widely in modern chemistry it will serve to alert senior chemists to those developments which will become routine in coming decades It will also be of interest to the broad community of computational chemists who study chemical systems

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