

NEW EDITION

## Fundamentals of Crystallography

THIRD EDITION

**Carmelo Giacovazzo**, University of Bari, **Hugo Luis Monaco**, University of Verona, **Gilberto Artioli**, University of Padova, **Davide Viterbo**, University del Piemonte Orientale, 'A. Avogadro', **Marco Milanesio**, University del Piemonte Orientale, 'A. Avogadro', **Gastone Gilli**, University of Ferrara, **Paola Gilli**, University of Ferrara, **Giuseppe Zanotti**, University of Padova, **Giovanni Ferraris**, University of Torino, and **Michele Catti**, University of Milano Bicocca

'... there is a good balance achieved between well-illustrated description and mathematical rigour. Established crystallographers will find it a handy reference manual, while at the same time the text remains accessible and informative reading for undergraduates with an interest in crystallography.'

The Times Higher Education Supplement

Crystallography is a basic tool for scientists in many diverse disciplines. This book offers a clear description of fundamentals and of modern applications. It will support curricula in crystallography at undergraduate level, contains material for advanced and specialized courses, and offers tools and ideas for courses in other disciplines.

International Union of Crystallography Texts on Crystallography No. 15

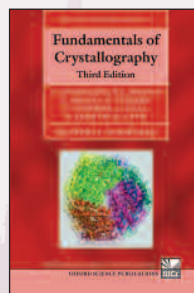
February 2011 | 872 pages | 482 b/w line and halftone illustrations | plus accompanying graphics on web site

978-0-19-957366-0, PAPERBACK

£45.00/\$82.50

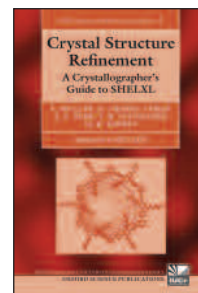
978-0-19-957365-3, HARDBACK

£90.00/\$162.00



## Crystal Structure Refinement

A Crystallographer's Guide to SHELXL



**Peter Muller**, MIT, **Regine Herbst-Imer**, University of Gottingen, **Anthony Spek**, Utrecht University, **Thomas Schneider**, FIRC Institute of Molecular Oncology, and **Michael Sawaya**, University of California, Los Angeles

This book is a mixture of textbook and tutorial. As a guide to SHELXL it covers advanced aspects of practical crystal structure refinement. In each of the chapters the book gives examples, describing every problem in detail. It comes with a CD-ROM with all files necessary to reproduce the refinements.

International Union of Crystallography Texts on Crystallography No. 8

2006 | 232 pages | 76 line drawings and 4 halftones

978-0-19-857076-9, HARDBACK

£59.95/\$140.00

## Symmetry in Crystallography

Understanding the International Tables

**Paolo Radaelli**, Oxford University

A fresh approach to teaching crystallographic symmetry. Rather than being swamped by heavy algebraic notation, the reader is taken through a series of simple and beautiful examples from the visual arts, and taught how to analyse them employing the 'pictorial' diagrams used in the International Tables of Crystallography.

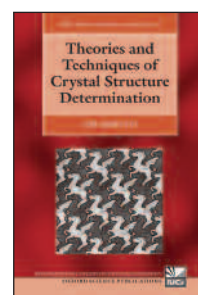
International Union of Crystallography Texts on Crystallography No. 16

June 2011 | 148 pages | 72 b/w line and halftone illustrations

978-0-19-955065-4, HARDBACK

£49.95/\$95.00

## Theories and Techniques of Crystal Structure Determination



**Uri Shmueli**, Tel Aviv University

'The real strength of this book lies in the way it condenses and modernizes the material of the classic texts.'

Acta Crystallographica

Solutions manual available for lecturers. Please visit [www.oup.com/uk](http://www.oup.com/uk) for more information.

International Union of Crystallography Monographs on Crystallography No. 9

2007 | 288 pages | 38 b/w line drawings | 2 b/w halftones and 1 colour plate

978-0-19-921966-7, PAPERBACK

£37.50/\$75.00

978-0-19-921350-4, HARDBACK

£77.50/\$150.00

## Aperiodic Crystals

From Modulated Phases to Quasicrystals



**Ted Janssen**, University of Nijmegen, **Gervais Chapuis**, Ecole Polytechnique Federale de Lausanne, and **Marc de Boissieu**, CNRS researcher, Laboratoire de Thermodynamique Physico Chimie Metallurgique, Grenoble

Most materials and crystals have an atomic structure which is described by a regular stacking of a microscopic fundamental unit, the unit cell. However, there are also many well-ordered materials without such a unit cell. This book deals with the structure determination and a discussion of the main special properties of these materials.

International Union of Crystallography Monographs on Crystallography No. 20

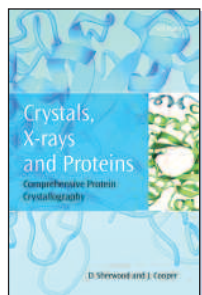
2007 | 480 pages | 163 b/w line drawings | 59 halftones

978-0-19-856777-6, HARDBACK

£89.95/\$180.00

## Crystals, X-rays and Proteins

Comprehensive Protein Crystallography



**Dennis Sherwood**, The Silver Bullet Machine Manufacturing Company, and **Jon Cooper**, University College, London

*Crystals, X-rays and Proteins* presents a complete account of the theory of the diffraction of X-rays by crystals with particular reference to the processes of determining the structures

of protein molecules. The book, which may be used at any post-school level, develops from first principles all relevant mathematics, diffraction and wave theory, and assumes no mathematical knowledge beyond integral calculus.

November 2010 | 640 pages | 250 b/w line and halftone illustrations

978-0-19-955904-6, HARDBACK

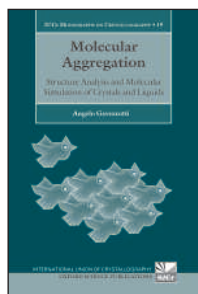
£55.00/\$98.50

Winner of the 2007 Trueblood Award of the American Crystallographic Association



## Molecular Aggregation

Structure analysis and molecular simulation of crystals and liquids



**Angelo Gavezzotti**, University of Milan

'Original and very topical, touching on the areas of molecular structure analysis, applied quantum theory, intermolecular forces, molecular dynamics, all with emphasis on the condensed states of matter.'

Jack Dunitz, ETH Zurich

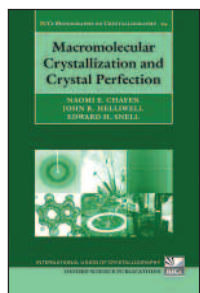
International Union of Crystallography Monographs on Crystallography No. 19

2006 | 448 pages | 140 line drawings | 5 halftones tables | OUP/International Union of Crystallography

978-0-19-857080-6, HARDBACK

£87.50/\$150.00

## Macromolecular Crystallization and Crystal Perfection



Available in  Available in...  
**Naomi E. Chayen**, Imperial College London, **John R. Helliwell**, University of Manchester, and **Edward H. Snell**, Hauptman-Woodward Institute, SUNY-Buffalo

'The book provides not only the key basic facts, but also provides the reader with the essential information to investigate further. It is timely and informative and certainly ought to be widely read by a range of different scientists with interests in macromolecular structure.'

Chemistry World

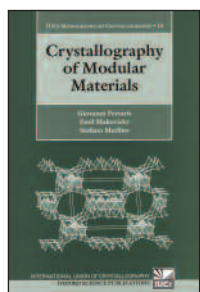
Structural biology is key to our understanding of the mechanisms of biological processes. This book describes current methods and future frontiers in crystal growth and use of X-ray and Neutron crystallography, in the context of the very successful current automation of crystallization and generation of synchrotron X-ray and neutron beams.


International Union of Crystallography Monographs on Crystallography No. 24

March 2010 | 240 pages | 33 line illustrations | 31 halftones  
 978-0-19-921235-2, HARDBACK £65.00/\$125.00

AVAILABLE IN PAPERBACK

## Crystallography of Modular Materials



Available in  Available in...  
**Giovanni Ferraris**, University of Turin, **Emil Makovicky**, University of Copenhagen, and **Stefano Merlino**, University of Pisa

This comprehensive text is addressed at scientists who are interested in considering crystalline materials from a non-conventional but inspiring viewpoint. The book contains the first

systematic theoretical and illustrative presentation of crystalline materials built from modules (including twinning) which determine and tune basic and technological properties.

International Union of Crystallography Monographs on Crystallography No. 15

2008 | 384 pages | numerous figures and tables  
 978-0-19-954569-8, PAPERBACK £44.50/\$74.00  
 978-0-19-852664-3, HARDBACK £115.00/\$199.00

NEW EDITION

## Crystal Structure Analysis

A Primer

THIRD EDITION

Edited by **Jenny Pickworth Glusker**, Fox Chase Cancer Centre and University of Pennsylvania, Philadelphia, and **Kenneth N. Trueblood**, University of California, Los Angeles

This book aims to explain how and why the detailed three-dimensional architecture of molecules can be determined by an analysis of the diffraction patterns obtained when X rays or neutrons are scattered by the atoms in single crystals. Part I deals with the nature of the crystalline state, diffraction generally, and diffraction by crystals in particular, and, briefly, the experimental procedures that are used. Part II examines the problem of converting the experimentally obtained data into a model of the atomic arrangement that scattered these beams. Part III is concerned with the techniques for refining the approximate structure to the degree warranted by the experimental data. It also describes the many types of information that can be learned by modern crystal structure analysis.

International Union of Crystallography Texts on Crystallography No. 14

May 2010 | 304 pages | 107 b&w line and halftone illustrations

978-0-19-957635-7, PAPERBACK £27.50/\$69.95  
 978-0-19-957634-0, HARDBACK £55.00/\$129.00



 suitable as a student text

NEW EDITION

## Crystal Structure Analysis

Principles and Practice

SECOND EDITION

Edited by **William Clegg**, University of Newcastle upon Tyne, **Alexander J Blake**, University of Nottingham, **Jacqueline M Cole**, University of Cambridge, **John S.O. Evans**, University of Durham, **Peter Main**, University of York, **Simon Parsons**, University of Edinburgh, and **David J Watkin**, University of Oxford

'Offers a balanced and readable overview and background of the subject as an entry point to understand and/or perform a single crystal structure analysis. As such, I can highly recommend this book as a companion to a hands-on course around one of the available structure determination software packages.'

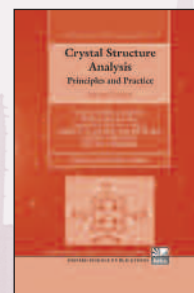
Tom Spek, *Crystallography Reviews*


This text focuses on the practical aspects of crystal structure analysis, and provides the necessary conceptual framework for understanding and applying the technique. Much of the material of the first edition has been significantly updated and expanded, and some new topics have been added. The approach to several of the topics has changed, reflecting recent developments in the subject.

International Union of Crystallography Texts on Crystallography No. 13

2009 | 408 pages | 140 line drawings and halftones

978-0-19-921947-6, PAPERBACK £33.50/\$59.95  
 978-0-19-921946-9, HARDBACK £67.50/\$120.00



 suitable as a student text

## The Nature of the Hydrogen Bond

Outline of a Comprehensive Hydrogen Bond Theory

Edited by **Gastone Gilli** and **Paola Gilli**, both at the University of Ferrara, Italy

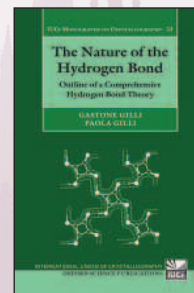
This book defines, for the first time, the rules for predicting H-bond energies and geometries from the properties of the interacting molecules. This new knowledge is used to investigate the molecular mechanisms in systems relevant to chemistry, biochemistry, pharmacology, crystallography, and material sciences where H-bonds have been shown to play a prominent role.

International Union of Crystallography Monographs on Crystallography No. 23

2009 | 336 pages | 120 b&w line drawings and 4-page colour plate section

978-0-19-955896-4, HARDBACK £67.50/\$130.00

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NEW EDITION

## The Basics of Crystallography and Diffraction

THIRD EDITION

Christopher Hammond, University of Leeds

'This is a very well-established student text. The author's style of presentation is lucid and the book contains some excellent exercises to 'stretch' the minds of students needing to acquire a facility with crystallography and diffraction.'

Materials Characterization

'The Basics of Crystallography and Diffraction brings a lot of classical information together into one place, and presents it in a way acceptable to a modern audience. It is well-structured, carefully written and a pleasure to read. There should be a copy on the shelves of every crystallography laboratory.'

ACA RefleXions

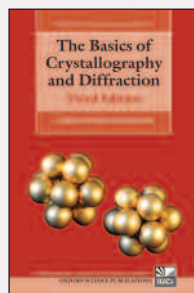
Crystallography and diffraction are widely used throughout many branches of science for studying structure. However, many students find these subjects abstruse and difficult. The aim of this book is to show, through relevant examples and without relying on complex mathematics, that the basic ideas behind crystallography and diffraction are simple and easily comprehensible. It is written by an experienced teacher with the needs of the student to the fore.

International Union of Crystallography Texts on Crystallography No. 12

2009 | 448 pages | 217 line drawings | 55 photographs

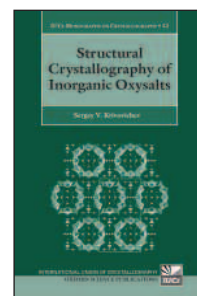
978-0-19-954645-9, PAPERBACK  
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£60.00/\$120.00



## Structural Crystallography of Inorganic Oxyalts

Available in...



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Inorganic oxyalts are chemical compounds that contain oxygen—the most abundant element in the Earth's core. Their atomic arrangement (crystal structure) has a dramatic influence upon their properties and, as a

consequence, upon the inorganic part of the world around us. This book is the first systematic survey of structures of inorganic oxyalts considered from the viewpoint of modern scientific methods of description and visualization of complex atomic arrangements.

International Union of Crystallography Monographs on Crystallography No. 22

2009 | 328 pages | 197 figures

978-0-19-921320-7, HARDBACK

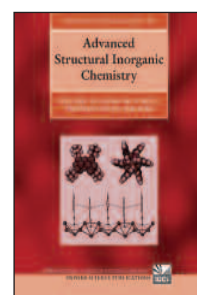
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## Advanced Structural Inorganic Chemistry

Available in...



Wai-Kei Li, The Chinese University of Hong Kong, Gong-Du Zhou, Peking University, and Thomas Mak, The Chinese University of Hong Kong



'In summary, the readers will find the many aspects of this book—a comprehensive textbook about chemical bonds, group theory and crystallography, descriptive and supramolecular inorganic chemistry—to be very useful. It is an important text for teaching inorganic chemistry.'

Coordination Chemistry Reviews

International Union of Crystallography Texts on Crystallography No. 10

2008 | 848 pages | 700 b&w line drawings  
30 b/w halftones

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978-0-19-921694-9, HARDBACK

£41.50/\$75.00  
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## Polymorphism in Molecular Crystals

Available in...



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'Clear, vigorous, well-written and very readable ... Joel Bernstein's book represents the single most important source for the development of critical understanding of polymorphism and its commercial and industrial importance.'

Current Engineering Practice

International Union of Crystallography Monographs on Crystallography No. 14

2007 | 424 pages | 280 line drawings and diagrams  
20 halftones | 4pp colour plates

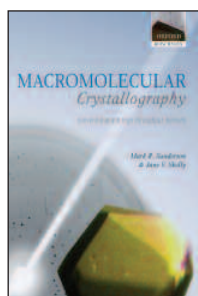
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## Macromolecular Crystallography

Conventional and high-throughput methods

Available in...



Edited by Mark R. Sanderson, King's College London, and Jane V. Skelly, University of Greenwich

'It is more than successful, and most, if not all, who dip into it will be rewarded by learning things they did not know, or possibly had forgotten ... a book that will surely find its place in every crystallographic lab whether protein or macromolecular.'

Lindsay Sawyer, Crystallography News

2007 | 304 pages | numerous halftones and line figures

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## Crystalline Molecular Complexes and Compounds

Structures and Principles

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Frank H. Herbstein, Israel Institute of Technology, Haifa

'This work is an absolute 'must purchase' for every chemical crystallography laboratory. The study of intermolecular assemblies and forces is probably now the number one topic in crystal chemistry and chemical crystallography, and any worker in the field, from beginning graduate student to experienced practitioner will find this work utterly invaluable.'

Crystallography Reviews

International Union of Crystallography Monographs on Crystallography No. 18

2005 | 1,352 pages | Numerous tables | figures and line drawings

978-0-19-852660-5, HARDBACK

£169.95/\$305.00

## Incommensurate Crystallography

Sander van Smaalen, University of Bayreuth, Germany

This book fully describes the structures and symmetries of incommensurately modulated crystals and composite crystals. It provides a complete presentation of crystallographic methods of structural analysis in incommensurate crystals, providing the necessary background for a skilled application of superspace methods to aperiodic crystals.

International Union of Crystallography Monographs on Crystallography No. 21

2007 | 284 pages | 96 figures

978-0-19-857082-0, HARDBACK

£75.00/\$150.00

## Crystallography of the Polymethylene Chain

An Inquiry into the Structure of Waxes

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Douglas L. Dorset, ExxonMobil Research and Engineering Co., Annandale, New Jersey

'The author brings together a huge amount of literature to provide a coherent and comprehensive account of the research area as it stands today. The overall presentation, including plentiful diagrams and photographs, is excellent—it is a worthy addition to the series.'

Crystallography News

International Union of Crystallography Monographs on Crystallography No. 17

2004 | 244 pages | numerous line figures and halftones

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£110.00/\$255.00

NEW IN PAPERBACK

**Structure Determination from Powder Diffraction Data**



Edited by **W.I.F. David**, ISIS Facility, Rutherford Appleton Laboratory, Didcot, **K. Shankland**, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, **L.B. McCusker**, ETH Zurich, Switzerland, and **C. Bärlocher**, ETH Zurich, Switzerland

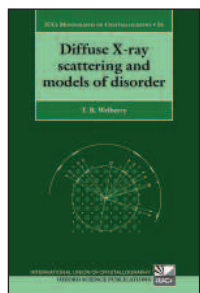
Our understanding of the properties of materials, from drugs and proteins to catalysts and ceramics, is almost always based on structural information. This book describes the developments in powder diffraction which make it possible for scientists to obtain such information, and guides both novices and practitioners through all the possibilities.

International Union of Crystallography Monographs on Crystallography No. 13

2006 | 360 pages | 96 line drawings and half tones  
 978-0-19-920553-0, PAPERBACK £49.95/\$99.00  
 978-0-19-850091-9, HARDBACK £115.00/\$199.00

NEW IN PAPERBACK

**Diffuse X-Ray Scattering and Models of Disorder**



**Thomas Richard Welberry**, Australian National University

Diffuse X-ray scattering is a rich source of local structural information over and above that obtained by conventional crystallography. The book aims to show how computer simulation of a model crystal provides a general method by which diffuse scattering

of all kinds and from all types of materials can be interpreted and analysed.

International Union of Crystallography Monographs on Crystallography No. 16

January 2010 | 280 pages | 180 line drawings and photographs  
 978-0-19-958381-2, PAPERBACK £37.50/\$65.00  
 978-0-19-852858-6, HARDBACK £99.95/\$175.00

**Applications of Neutron Powder Diffraction**



**Erich H. Kisi** and **Christopher J. Howard**, both at The University of Newcastle, Australia

'The Oxford series gained a reputation for being authoritative and, as far as the many aspects of neutron powder diffraction are concerned, newcomers will find all they need to guide them in applying the technique to their needs, whether they magnetism, amorphous materials or stress analysis.'

Peter Day, *Chemistry World*

Oxford Series on Neutron Scattering in Condensed Matter No. 15

2008 | 504 pages | 182 line figures | 8 b/w photographs  
 9 colour images  
 978-0-19-851594-4, HARDBACK £72.50/\$150.00

**Neutron Protein Crystallography**

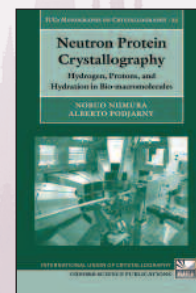
*Hydrogen, Protons, and Hydration in Bio-macromolecules*

**Nobuo Niimura**, Ibaraki University, Japan, and **Alberto Podjarny**, CNRS, France

One of the first books in the world dedicated to the emerging field of neutron protein crystallography (NPC). It covers all of the practical aspects of NPC, from the basic background of neutron scattering and diffraction, to the technical details of neutron facilities, growth of high-quality crystals, and data analysis. The final chapter is devoted to providing many examples of using NPC to investigate a wide range of different proteins. It demonstrates how NPC can explore hydrogen bonds, protonation and deprotonation of amino acid residues, hydration structures, and hydrogen-to-deuterium exchange ratios.

International Union of Crystallography Monographs on Crystallography No. 25

February 2011 | 232 pages | 150 b/w line and half tone illustrations  
 978-0-19-957886-3, HARDBACK



£65.00/\$45.00

**Diffuse Scattering and Defect Structure Simulations**



*A cook book using the program DISCUS*

**Reinhard B. Neder**, University of Erlangen-Nürnberg, Germany, and **Thomas Proffen**, Los Alamos National Laboratory, New Mexico

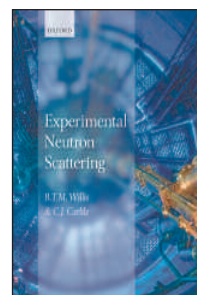
'This book admirably succeeds in providing a course of instruction particularly for students and postdoctoral workers wishing to enter the field of diffuse scattering. The DISCUS suite of programs is a powerful tool that is very accessible and together with the book provides an excellent basis for self-tuition as well as for handling many situations likely to be encountered in a research environment.'

Crystallography Reviews

International Union of Crystallography Texts on Crystallography No. 11

2008 | 240 pages | 103 line drawings and 32 b&w halftones  
 978-0-19-923369-4, HARDBACK £48.50/\$90.00

**Experimental Neutron Scattering**



**B. T. M. Willis**, University of Oxford, and **C. J. Carlile**, University of Lund

This book provides a broad survey of the work carried out by scientists at neutron centres around the world, which provide the facilities for generating intense beams of neutrons. These beams are essential in investigating the atomic structures of a wide

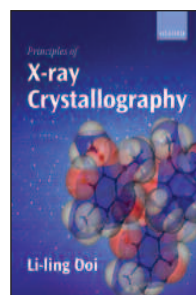
range of materials such as magnetic alloys, superconductors, polymers, or proteins.

2009 | 344 pages | 165 line drawings and 19 halftones  
 978-0-19-851970-6, HARDBACK £47.50/\$90.00

**Principles of X-ray Crystallography**



**Li-ling Ooi**, Formerly of Cardiff University



*Principles of X-ray Crystallography* provides a clear, succinct guide to the three-dimensional world of molecules, which is perfect for anyone encountering the technique for the first time. Using a direct and simple writing voice, and enriching the text with real examples, diagrams, exercises, and activities, it seeks to engage the reader in the challenge of

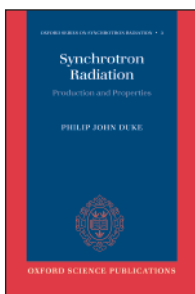
visualizing three-dimensional structures, rather than daunting them with excessive theoretical detail.

2009 | 176 pages | 110 halftones  
 978-0-19-956904-5, PAPERBACK £21.99/\$39.95

NEW IN PAPERBACK

**Synchrotron Radiation**

*Production and Properties*



**Philip Duke**, Daresbury Laboratory

'Those who do wonder about the origins of synchrotron radiation will find P.J. Duke's book a valuable and thorough source of facts describing its physical basis from first principles. The reader sees the elaborate production and remarkable properties of synchrotron

radiation unfolded within merely 251 pages and 15 chapters. More than forty years of experience in the field qualify the author to educate an international interdisciplinary community of synchrotron radiation users.'

Journal of Synchrotron Radiation

Oxford Series on Synchrotron Radiation No. 3

2008 | 272 pages | 2 halftones and numerous line illustrations  
 978-0-19-955909-1, PAPERBACK £32.50/\$60.00

HAVE YOU SEEN?

**Dove:** *Structure and Dynamics* on page 4 in Oxford Master Series