

Structure determination from powder diffraction data. International Union of Crystallography Monographs in Crystallography. No. 13. Edited by W. I. F.

David, K. Shankland, L. B. McCusker and Ch. Baerlocher. Pp. xix + 337. Oxford University Press, 2006. Price (paperback) GBP 39.95. ISBN 978-0-19-920553-0.

The art of solving a structure from powder diffraction data has developed rapidly over the last ten years to the point where numerous crystal structures, both organic and inorganic, have been solved directly from powder data. However, it is still an art and, in contrast to its single-crystal equivalent, is far from routine. The art lies not only in the correct application of a specific experimental technique or computer program but also in the selection of the optimal path for the problem at hand. Written and edited by experts active in the field, and covering both the fundamental and applied aspects of structure solution from powder diffraction data, this book guides both novices and experienced practitioners alike through the maze of possibilities. *Readership:* Graduate students, lecturers and researchers in crystallography, physical chemistry, and materials science; all practitioners of powder diffraction in academia and industry; chemists and chemical analysts in the chemical, materials, and pharmaceutical industry. *Contents:* 1. Introduction, 2. Structure determination from powder diffraction data: an overview, 3. Laboratory X-ray powder diffraction, 4. Synchrotron radiation powder diffraction, 5. Neutron powder diffraction, 6. Sample preparation, instrument selection and data collection, 7. Autoindexing, 8. Extracting integrated intensities from powder diffraction patterns, 9. Experimental methods for estimating the relative intensities of overlapping reflections, 10. Direct methods in powder diffraction – basic concepts, 11. Direct methods in powder diffraction – applications, 12. Patterson methods in powder diffraction: maximum entropy and symmetry minimum function techniques, 13. Solution of Patterson-type syntheses with

books received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty finding a suitable reviewer without great delay.

the direct methods sum function, 14. A maximum entropy approach to structure solution, 15. Global optimization strategies, 16. Solution of flexible molecular structures by simulated annealing, 17. Chemical information and intuition in solving crystal structures.

Structure and chemistry of crystalline

solids. By B. E. Douglas and S.-M. Ho. Pp. x + 346. New York: Springer Science and Business Media, 2006. Price (hardback) EUR 99.95, USD 129.00, GBP 77.00. ISBN 978-0-387-26147-8.

Most chemists, metallurgists, mineralogists, geologists and workers in material sciences need a simple system and notation for describing crystal structures. *Structure and chemistry of crystalline solids* presents a widely applicable system with simple notation giving important information about the structure and the chemical environment of ions or molecules. It is easily understood and used by those concerned with applications dependent on structure–property relationships. Insight into crystal structures, including some complex silicates, is aided by the use of the *CrystalMaker* computer program. The bundled CD-ROM, which uses *CrystalMaker* for instruction and demos on both Windows and Macintosh platforms, allows the user to manipulate the structures. *Written for:* chemists, materials scientists, metallurgists, mineralogists and geologists, graduate students in solid-state chemistry and related areas in materials science. *Contents:* 1. Introduction, 2. Classification of crystals, point groups and space groups, 3. Close packing and the PTOT System, 4. Crystal structures of the elements, 5. Crystal structures involving P and O layers, 6. Crystal structures involving P and T layers, 7. Crystal structures involving P, T and O layers, 8. Crystal structures with multiple layers, 9. Crystal structures of some intermetallic compounds, 10. Crystal structures of silica and metal silicates, 11. Crystal structures of organic compounds, 12. Predicting structures and assigning notations.

Handbook of X-ray data. By G.

Zschornack. Pp. IX + 967. Berlin: Springer-Verlag, 2007. Price (hardback) EUR 213.95. ISBN 978-3-540-28618-9.

This sourcebook is intended as an X-ray data reference for scientists and engineers working in the field of energy- or wavelength-dispersive X-ray spectrometry and related fields of basic and applied research, technology, or process and quality controlling. In a concise and informative manner, the most important data connected with the emission of characteristic X-ray lines are tabulated for all elements up to $Z = 95$ (americium). This includes X-ray energies, emission rates and widths as well as level characteristics such as binding energies, fluorescence yields, level widths and absorption edges. The tabulated data are characterized and, in most cases, evaluated. Furthermore, all important processes and phenomena connected with the production, emission and detection of characteristic X-rays are discussed. This reference book addresses all researchers and practitioners working with X-ray radiation and fills a gap in the available literature. *Contents:* Part I: Atomic structure, X-ray physics and radiation detection; 1. X-ray physics and practice, 2. Physical fundamentals, 3. Energy and intensity measurements, 4. Data base; Part II: X-ray reference data; 5. X-ray emission lines and atomic level characteristics, 6. X-ray transition energies ordered by energy/wavelength, 7. K -shell intensity ratios and K -vacancy decay rates, 8. Atomic scattering factors, 9. Analytical approximation of atomic scattering factors, 10. Mass attenuation coefficients, 11. Fit parameters for the calculation of mass attenuation coefficients, 12. Atomic weights and isotope masses, 13. Parameters of stable isotopes, 14. Parameters of long-live radioactive isotopes, 15. Mean X-ray transition energies. 588 references.