



Modern Crystallography I (Springer Series in Solid-State Sciences)

Vainshtein, B. K.

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Modern Crystallography

L.A. Shuvalov



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and geometric representations in the theory of crystal structure and crystal chemistry as well as lattice energy are considered. The important classes of crystal structures in inorganic compounds as well as the structure polymers, liquid crystals, biological crystals and macromolecules are treated. This second edition is complemented with recent data on many types of crystal structures: fullerenes, high temperature superconductors, minerals, liquid crystals, etc.

Phasing in Crystallography Carmelo Giacovazzo, 2013-12-12. Modern crystallographic methods originate from the synergy of two main research streams: the small molecule and the macro molecular streams. The first stream was able to definitively solve the phase problem for molecules up to 200 atoms in the asymmetric unit. The achievements obtained by the macromolecular stream are also impressive. A huge number of protein structures have been deposited in the Protein Data Bank. The solution of them is no longer reserved to an elite group of scientists but may be attained in a large number of laboratories around the world even by young scientists. New probabilistic approaches have been tailored to deal with larger structures, errors in the experimental data and modest data resolution. Traditional phasing techniques like *ab initio* molecular replacement, isomorphous replacement and anomalous dispersion techniques have been revisited. The new approaches have been implemented in robust phasing programs which have been organized in automatic pipelines usable even by non experts. Protein structures which 50 years ago could take months or even years to solve can now be solved in a matter of hours, partly also due to technological advances in computer science. This book describes all modern crystallographic phasing methods and introduces a new rational classification of them. A didactic approach is used with the techniques described simply and logically in the main text and further mathematical details confined to the Appendices for motivated readers. Numerous figures and applicative details illustrate the text.

Crystal Symmetries B. K. Vainshtein, I. Hargittai, 2017-07-26. *Crystal Symmetries* is a timely account of the progress in the most diverse fields of crystallography. It presents a broad overview of the theory of symmetry and contains state of the art reports of its modern directions and applications to crystal physics and crystal properties. Geometry takes a special place in this treatise. Structural aspects of phase transitions, correlation of structure and properties, polytypism, modulated structures and other topics are discussed. Applications of important techniques such as X-ray crystallography, biophysical studies, EPR spectroscopy, crystal optics and nuclear solid state physics are represented. Contains 30 research and review papers.

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