



Crystal Structure Determination

By Werner Massa

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This textbook gives a concise introduction to modern crystal structure determination, emphasising both its theoretical background and the way it is actually carried out. The theoretical sections are supported by many illustrations, and lay emphasis on a good understanding rather than rigorous mathematics. The most important data collection techniques, and the methods of data reduction, structure solution and refinement are discussed from a practical point of view. Many tips and insights help readers to recognise and avoid possible errors and traps, and to judge the quality of results. The second edition has been considerably updated, especially the chapter on experimental methods, which is now mainly concerned with modern data collection using area-detectors.

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"The book provides a nice balance between describing the mathematical fundamentals and offering practical advice on how to solve a crystal structure... appropriate for an undergraduate audience (particularly in chemistry) and for graduate students or researchers who find they need a better grasp of the subject... a very helpful addition to the collection of introductory texts in X-ray crystallography. Especially for its treatment of common errors in the collection of intensity data and in the interpretation of results."

Acta Crystallographica

"Details at great length the inherent pitfalls and errors that one may encounter when calculating crystal structures using new software programs. The author does an excellent job of describing these errors and ways to recognize them when they appear in your calculations." *Mineralium Deposita*

From the reviews of the second edition:

"This textbook gives a concise introduction to modern crystal structure determination The theoretical sections are supported by many illustrations, and lay emphasis on a good understanding The most important data collection techniques ... are discussed from a practical point of view. Many tips and insights help readers to recognise and avoid possible errors and traps, and to judge the quality of results." (*Chimie Nouvelle Societe Royale de Chimie*, Vol. 23 (89), juin, 2005)

“‘Crystal Structure Determination’ gives a concise introduction to the subject, with particular emphasis placed on the manner in which contemporary analysis actually occurs. ... The strengths of this book are numerous. The presentation is excellent: the diagrams are plentiful and often impressive, and the formatting of the text is very pleasing to the eye. ... the research chemist with a desire to appreciate more fully a technique that they are likely to use with increasing frequency – the book should be a helpful companion.” (Andrew Bond, *Crystallography News*, June, 2004)

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