
Preface to the Fifth Edition

We were honoured to be asked by Springer, New York to prepare a fifth edition of *Structure Determination by X-ray Crystallography*. First published in 1977 under the Plenum imprint, this book has received wide acclaim in both teaching and research in X-ray crystallography because of its extensive and detailed coverage of all aspects of the subject.

As we prepare this new edition, we are entering the centenary of the discovery of X-ray diffraction in 1912, the beginning of X-ray crystallography as a science in its own right. Today, X-ray crystallography and the complementary technique of neutron diffraction together provide the most powerful tools for the investigation and elucidation of crystal and molecular structures. X-ray and neutron crystallography may be described as the science of the structure of materials, in the widest sense of the phrase, and their ramifications are evident across a broad spectrum of scientific endeavour.

The power of computers and available software has unleashed an unprecedented ability to carry out with speed the complicated calculations involved in crystal structure determination on a desktop PC. This is paralleled by the availability of powerful X-ray and neutron sources and low temperature devices for facilitating measurements at liquid nitrogen temperature or lower, which provide ever higher precision in the determination of crystal structures. However, a detailed knowledge of the theory underlying the process of crystal structure determination is still required in order both to ensure that the literature contains correct well-determined structures and to understand the complexities introduced by features such as disorder and twinning in crystals. There are many pitfalls in crystal structure determination to trap the unwary.

In this new edition, we have continued the approach that has been well reviewed in its earlier editions. We have always kept in mind that students meeting X-ray crystallography for the first time are encountering a new discipline, and not merely extending the range of a subject already studied. In consequence, we have chosen, for example, to discuss the geometry and symmetry of crystals in rather more detail than is found in other books on this subject, for it is our experience that some of the difficulties that students meet in introductory X-ray crystallography lie in their unfamiliarity with a three-dimensional concept, whether they be final-year undergraduate or post-graduate students in chemistry, biochemistry, materials science, geology, bioinformatics, information technology, or physics. Both low molecular weight (small molecules) and macromolecular methods (proteins) are covered in detail.

As well as retaining and thoroughly revising the overall contents of the earlier editions, we have added a significant chapter on neutron diffraction studies, and sections introducing Molecular Modelling and Structure Prediction. In order to maintain a workable size for the book, a number of elaborations of mainly mathematical argument have been stored as Web Appendices on the website <http://extras.springer.com>.

Although several novel methods have been added to the armoury of crystal structure determination, we limit our discussion principally to Patterson interpretation, Direct Methods, Isomorphous and Molecular Replacement and Powder Crystallography, and developments from them. The basic problem remains the determination of the phases of X-ray reflections, and this problem is addressed in these techniques discussed herein. In order to simulate the actual process of structure determination, we are fortunate to be able to include the XRAY program package prepared by Dr. Neil Bailey and colleagues of the University of Sheffield, and we are grateful to him for permission to use it in the present context. It has been modified (M.L.) for PC operation and several enhancements made, including the presentation of Fourier contour maps on the monitor. Although this package uses two-dimensional data, much valuable insight into X-ray structure determination can be gained, and a number of sets of X-ray data are included.

There are now numerous computer packages available for the many aspects of crystallography that are in current use. We have referred to them freely within the text, and they have been collected in an appendix together with a reference to a source for each so that they become readily available to the practising crystallographer. There are numerous references to each chapter including website addresses for topics of crystallographic importance. References among the text are given as “Sect. 1.2.3,” which refers to that section in Chap. 1, or as “(3.4)” which refers to that equation in Chap. 3.

Each chapter contains a set of problems designed to assist the reader in the understanding of the textual material, and detailed tutorial solutions are provided. Some of these problems require computer assistance, and a set of programs has been designed and included with the Web material and dated 1 January 2013 (Version 5.1). In this context, we are grateful to Dr. Jan Visser of the Technisch Fysische Dienst, Delft, Professor Armel Le Bail of Laboratoire Fluorures, Université du Maine, Le Mans, and Professor A L Spek of the University of Utrecht for the continued incorporation of the programs ITO12, ESPOIR, and LEPAGE, respectively, in the Program Suite for this book. Finally we thank Springer Science + Business Media for inviting this edition and bringing it to a state of completion.

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Analysis by X-rays and Neutrons

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