
Preface to the Second English Edition

The second English edition is largely based on the third German edition of the Teubner Studienbuch “Kristallstrukturbestimmung,” which appeared in 2002. In particular, Chapter 7, dealing with experimental methods, has been extensively rewritten. In view of the huge recent advances in the use of area detector systems for single-crystal data collection, their description has replaced much of the material on “classic” methods. Similarly, the practical example (Chapter 15) now describes area-collector methods more fully. Among many other cases, the sections on Rietveld refinement, macromolecular crystallography and uses of databases have been updated. I am grateful to my colleague R.O. Gould for continuing his excellent translation of the first edition, and for the friendly and careful collaboration in achieving many large and small improvements.

Werner Massa

Marburg, November 2003

Preface to the First German Edition

Crystal structure analysis using X-rays has undergone an expansion of avalanche proportions in the last twenty years, thanks to the development of rapid and automatic means of data collection and the enormous growth of the computer hardware and software for carrying out the necessary calculations. Because of its wide applicability and its precision, it has become one of the most important tools in both organic and inorganic chemical research. Despite the fact that crystallography plays a very minor role in most undergraduate study, many students have found that in the course of graduate or even undergraduate research, they need to undertake a crystal structure determination themselves, or at least to become competent to interpret crystallographic results. Thanks to ever improving program systems, the many complex steps of a structure analysis are certainly becoming less and less difficult for the beginner to master. Nonetheless, regarding the process simply as a “black box” is fraught with danger.

This book is aimed at those students of chemistry and related subjects who wish to take a look into the black box before they step into its territory, or who simply wish to learn more of the fundamentals, the opportunities and the risks of the method. In view of the well-known fact that the likelihood a book will actually be read is inversely proportional to its number of pages, fundamentals of the method are treated here as briefly and as intuitively as possible. It seems more important that chemists should have a grasp of the basic principles and their application to a problem, than that they be in a position to understand fully the complex mathematical formalisms employed by the computer programs.

On the other hand, some aspects of the subject, which bear directly on the quality of a structure determination, are worth fuller treatment. These include discussion of a number of significant errors and the recognition and treatment of disorder and

twinning. Most important crystallographic literature is available in English, but a few references in other languages, principally German, have been included.

This book is based in part on lectures and on a seminar at the University of Marburg. Consciously or unconsciously, many colleagues have made their contributions. I am particularly grateful to Professor D. Babel for many helpful suggestions and a critical reading of the manuscript. I thank Dr. K. Harms for proofreading the manuscript and Mr. C. Frommen for considerable assistance with the production of camera-ready copy using the \LaTeX program. Finally, I acknowledge the help of my wife Hedwig and my children for all their assistance and patience during the preparation of this book.

Werner Massa

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Massa, W.

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