

## Preface

BY URI SHMUELI

The purpose of Volume B of *International Tables for Crystallography* is to provide the user or reader with accounts of some well established topics, of importance to the science of crystallography, which are related in one way or another to the concepts of reciprocal lattice and, more generally, reciprocal space. Efforts have been made to extend the treatment of the various topics to include X-ray, electron, and neutron diffraction techniques, and thereby do some justice to the inclusion of the present Volume in the new series of *International Tables for Crystallography*.

An important crystallographic aspect of symmetry in reciprocal space, space-group-dependent expressions of trigonometric structure factors, already appears in Volume I of *International Tables for X-ray Crystallography*, and preliminary plans for incorporating this and other crystallographic aspects of reciprocal space in the new edition of *International Tables* date back to 1972. However, work on a volume of *International Tables for Crystallography*, largely dedicated to the subject of reciprocal space, began over ten years later. The present structure of Volume B, as determined in the years preceding the 1984 Hamburg congress of the International Union of Crystallography (IUCr), is due to (i) computer-controlled production of concise structure-factor tables, (ii) the ability to introduce many more aspects of reciprocal space – as a result of reducing the effort of producing the above tables, as well as their volume, and (iii) suggestions by the National Committees and individual crystallographers of some additional interesting topics. It should be pointed out that the initial plans for the present Volume and Volume C (*Mathematical, Physical and Chemical Tables*, edited by Professor A. J. C. Wilson), were formulated and approved during the same period.

The obviously delayed publication of Volume B is due to several reasons. Some minor delays were caused by a requirement that potential contributors should be approved by the Executive Committee prior to issuing relevant invitations. Much more serious delays were caused by authors who failed to deliver their contributions. In fact, some invited contributions had to be excluded from this first edition of Volume B. Some of the topics here treated are greatly extended, considerably updated or modern versions of similar topics previously treated in the old Volumes I, II, and IV. Most of the subjects treated in Volume B are new to *International Tables*.

I gratefully thank Professor A. J. C. Wilson, for suggesting that I edit this Volume and for sharing with me his rich editorial experience. I am indebted to those authors of Volume B who took my requests and deadlines seriously, and to the Computing Center of Tel Aviv University for computing facilities and time. Special thanks are due to Mrs Z. Stein (Tel Aviv University) for skilful assistance in numeric and symbolic programming, involved in my contributions to this Volume.

I am most grateful to many colleagues—crystallographers for encouragement, advice, and suggestions. In particular, thanks are due to Professors J. M. Cowley, P. Goodman and C. J. Humphreys, who served as Chairmen of the Commission on Electron Diffraction during the preparation of this Volume, for prompt and expert help at all stages of the editing. The kind assistance of Dr J. N. King, the Executive Secretary of the IUCr, is also gratefully acknowledged. Last, but certainly not least, I wish to thank Mr M. H. Dacombe, the Technical Editor of the IUCr, and his staff for the skilful and competent treatment of the variety of drafts and proofs out of which this Volume arose.

## Preface to the second edition

BY URI SHMUELI

The first edition of Volume B appeared in 1993, and was followed by a corrected reprint in 1996. Although practically all the material for the second edition was available in early 1997, its publication was delayed by the decision to translate all of Volume B, and indeed all the other volumes of *International Tables for Crystallography*, to Standard Generalized Markup Language (SGML) and thus make them available also in an electronic form suitable for modern publishing procedures.

During the preparation of the second edition, most chapters that appeared in the first edition have been corrected and/or revised, some were rather extensively updated, and five new chapters were added. The overall structure of the second edition is outlined below.

After an introductory chapter, Part 1 presents the reader with an account of structure-factor formalisms, an extensive treatment of the theory, algorithms and crystallographic applications of Fourier methods, and treatments of symmetry in reciprocal space. These are here enriched with more advanced aspects of representations of space groups in reciprocal space.

In Part 2, these general accounts are followed by detailed expositions of crystallographic statistics, the theory of direct methods, Patterson techniques, isomorphous replacement and anomalous scattering, and treatments of the role of electron

microscopy and diffraction in crystal structure determination. The latter topic is here enhanced by applications of direct methods to electron crystallography.

Part 3, *Dual Bases in Crystallographic Computing*, deals with applications of reciprocal space to molecular geometry and ‘best’-plane calculations, and contains a treatment of the principles of molecular graphics and modelling and their applications; it concludes with the presentation of a convergence-acceleration method, of importance in the computation of approximate lattice sums.

Part 4 contains treatments of various diffuse-scattering phenomena arising from crystal dynamics, disorder and low dimensionality (liquid crystals), and an exposition of the underlying theories and/or experimental evidence. The new additions to this part are treatments of polymer crystallography and of reciprocal-space images of aperiodic crystals.

Part 5 contains introductory treatments of the theory of the interaction of radiation with matter, the so-called dynamical theory, as applied to X-ray, electron and neutron diffraction techniques. The chapter on the dynamical theory of neutron diffraction is new.

I am deeply grateful to the authors of the new contributions for making their expertise available to Volume B and for their

## PREFACE

excellent collaboration. I also take special pleasure in thanking those authors of the first edition who revised and updated their contributions in view of recent developments. Last but not least, I wish to thank all the authors for their contributions and their patience, and am grateful to those authors who took my requests seriously. I hope that the updating and revision of future editions will be much easier and more expedient, mainly because of the new format of *International Tables*.

Four friends and greatly respected colleagues who contributed to the second edition of Volume B are no longer with us. These are Professors Arthur J. C. Wilson, Peter Goodman, Verner Schomaker and Boris K. Vainshtein. I asked Professors Michiyoshi Tanaka, John Cowley and Douglas Dorset if they were prepared to answer queries related to the contributions of the late Peter Goodman and Boris K. Vainshtein to Chapter 2.5. I am most grateful for their prompt agreement.

This editorial work was carried out at the School of Chemistry and the Computing Center of Tel Aviv University. The facilities they put at my disposal are gratefully acknowledged on my behalf and on behalf of the IUCr. I wish to thank many colleagues for interesting conversations and advice, and in particular Professor Theo Hahn with whom I discussed at length problems regarding Volume B and *International Tables* in general.

Given all these expert contributions, the publication of this volume would not have been possible without the expertise and devotion of the Technical Editors of the IUCr. My thanks go to Mrs Sue King, for her cooperation during the early stages of the work on the second edition of Volume B, while the material was being collected, and to Dr Nicola Ashcroft, for her collaboration during the final stages of the production of the volume, for her most careful and competent treatment of the proofs, and last but not least for her tactful and friendly attitude.