

PREFACE

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.

Preface to the third edition

BY URI SHMUELI

The second edition of Volume B appeared in 2001. Plans for the third edition included the addition of new chapters and sections, the substantial revision of several chapters that existed in the second edition and minor revisions and updating of existing chapters. The overall structure of Volume B remained unchanged.

In Part 1, Chapter 1.5 on classifications of space-group representations in reciprocal space has been extensively revised.

In Part 2, Chapter 2.2 on direct methods has been considerably extended to include applications of these methods to macromolecular crystallography. Chapter 2.3 on Patterson and molecular replacement techniques has been updated and extended. Section 2.5.3 on convergent-beam electron diffraction has been completely rewritten by a newly invited author, and Section 2.5.6 on three-dimensional reconstruction has been updated and extended by a newly invited author, who has also added Section 2.5.7 on single-particle reconstruction. The Foreword to Chapter 2.5 on electron diffraction and microscopy has also been revised.

In Part 3, Chapter 3.3 on computer graphics and molecular modelling has been enriched by Section 3.3.4 on the implementation of molecular graphics to small and medium-sized molecules, and a comprehensive Chapter 3.5 on modern extensions of Ewald methods has been added, dealing with (i) inclusion of fast Fourier transforms in the computation of sums and (ii) departure from the point-charge model in Ewald summations.

In Part 4, Chapter 4.1 on thermal diffuse scattering of X-rays and neutrons has been updated, and Chapter 4.2 on disorder diffuse scattering of X-rays and neutrons has been extensively revised and updated.

Minor updates and corrections have also been made to several existing chapters and sections in all the parts of the volume.

My gratitude is extended to the authors of new contributions and to the authors of the first and second editions of the volume for significant revisions of their chapters and sections in view of new developments. I wish to thank all the authors for their excellent collaboration and for sharing with the *International Tables for Crystallography* their expertise. I hope that the tradition of keeping the contributions up to date will also persist in future editions of Volume B. This will be aided by significant improvements in various aspects of technical editing which were already apparent in the preparation of this edition.

Three greatly respected friends and colleagues who contributed to this and previous editions of Volume B passed away after the second edition of Volume B was published. These are Professors John Cowley, Boris Zvyagin and Donald Williams. I asked Professors John Spence, Douglas Dorset and Pawel Penczek to take care of any questions about the articles of the late John Cowley, Boris Zvyagin and Boris Vainshtein in Chapter 2.5, and Dr Bill Smith to answer any questions about Chapter 3.4 by the late Donald Williams. They all agreed promptly and I am most grateful for this.

My editorial work was carried out at the School of Chemistry of Tel Aviv University and I wish to acknowledge gratefully the facilities that were put at my disposal. I am grateful to many friends and colleagues for interesting conversations and exchanges related to this volume. Thanks are also due to my friends from the IUCr office in Chester for their helpful interest.

Finally, I think that the publication of the third edition of Volume B would not have been possible without the competent, tactful and friendly collaboration of Dr Nicola Ashcroft, the Technical Editor of this project during all the stages of the preparation of this edition.