position under consideration were selected from the stored list of all conceivable reflection conditions by the following procedure:

(1) All conditions which apply to at least one h, k, l triplet of the set with structure factor zero are deleted from the list of all conceivable reflection conditions,

(2) conditions which do not apply to at least one h, k, l triplet of the set with structure factor non-zero are deleted,

(3) redundant conditions are removed by ensuring that each h, k, l triplet with structure factor non-zero is described by one reflection condition only.

Finally the completeness of the resulting reflection conditions for the Wyckoff position was proved by verifying that for each h, k, l triplet with non-zero structure factor there is a reflection condition that describes it. If this turned out not to be the case the list of all conceivable reflection conditions stored in the program was evidently incomplete and had to be extended by the missing conditions, after which the procedure was repeated.

Fifth, Revised Edition, 2002

By M. I. Aroyo and P. B. Konstantinov

The computer production of the space-group tables in 1983 described above served well for the first and several subsequent editions of Volume A. With time, however, it became apparent that a modern, versatile and flexible computer version of the entire volume was needed (*cf. Preface* and *Foreword to the Fifth, Revised Edition*).

Hence, in October 1997, a new project for the electronic production of the Fifth Edition of Volume A was started. Part of this project concerned the computerization of the plane- and space-group tables (Part 6 and 7), excluding the space-group diagrams. The aim was to produce a PostScript file of the content of these tables which could be used for printing from and in which the layout of the tables had to follow exactly that of the previous editions of Volume A. Having the space-group tables in electronic form opens the way for easy corrections and modifications of later editions, as well as for a possible future electronic edition of Volume A.

The LaTeX document preparation system [Lamport, L. (1994). *A Document Preparation System*, 2nd ed. Reading, MA: Addison-Wesley], which is based on the TeX typesetting software, was used for the preparation of these tables. It was chosen because of its high versatility and general availability on almost any computer platform.

A separate file was created for each plane and space group and each setting. These 'data files' contain the information listed in the plane- and space-group tables and are encoded using standard LaTeX constructs. These specially designed commands and environments are defined in a separate 'package' file, which essentially contains programs responsible for the typographical layout of the data. Thus, the main principle of LaTeX – keeping content and presentation separate – was followed as closely as possible.

The final typesetting of all the plane- and space-group tables was done by a single computer job, taking 1 to 2 minutes on a modern workstation. References in the tables from one page to another were automatically computed. The result is a PostScript file which can be fed to a laser printer or other modern printing or typesetting equipment.

The different types of data in the LaTeX files were either keyed by hand or computer generated, and were additionally checked by specially written programs. The preparation of the data files can be summarized as follows:

Headline, *Origin*, *Asymmetric unit*: hand keyed.

Symmetry operations: partly created by a computer program. The algorithm for the derivation of symmetry operations from their matrix representation is similar to that described in the literature [*e.g.* Hahn, Th. & Wondratschek, H. (1994). *Symmetry of Crystals*. Sofia: Heron Press]. The data were additionally checked by automatic comparison with the output of the computer program *SPACER* [Stróż, K. (1997). *SPACER: a program to display space-group information for a conventional and nonconventional coordinate system. J. Appl. Cryst.* **30**, 178–181].

Generators: transferred automatically from the database of the forthcoming Volume A1 of *International Tables for Crystallography*, *Symmetry Relations between Space Groups* (edited by H. Wondratschek & U. Müller), hereafter referred to as *IT* A1.

General positions: created by a program. The algorithm uses the well known generating process for space groups based on their solvability property (H. Wondratschek, Part 8 of this volume).

Special positions: The first representatives of the Wyckoff positions were typed in by hand. The Wyckoff letters are assigned automatically by the TeX macros according to the order of appearance of the special positions in the data file. The multiplicity of the position, the oriented site-symmetry symbol and the rest of the representatives of the Wyckoff position were generated by a program. Again, the data were compared with the results of the program *SPACER*.

Reflection conditions: hand keyed. A program for automatic checking of the special-position coordinates and the corresponding reflection conditions with h, k, l ranging from -20 to 20 was developed.

Symmetry of special projections: hand keyed.

Maximal subgroups and minimal supergroups: most of the data were automatically transferred from the data files of *IT* A1. The macros for their typesetting were reimplemented to obtain exactly the layout of Volume A. The data of isomorphic subgroups (IIc) with indices greater than 4 were added by hand.

The contents of the LaTeX files and the arrangement of the data correspond exactly to that of previous editions of this volume with the following exceptions:

(i) Introduction of the glide-plane symbol '*e*' [Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Hahn, Th., Senechal, M., Shoemaker, D. P., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1992). *Symbols for symmetry elements and symmetry operations. Acta Cryst.* A**48**, 727–732] in the conventional Hermann–Mauguin symbols as described in Chapter 1.3, Note (x). The new notation was also introduced for some origin descriptions and in the nonconventional Hermann–Mauguin symbols of maximal subgroups.

(ii) Changes in the subgroup and supergroup data following the *IT* A1 conventions:

(1) Introduction of space-group numbers for subgroups and supergroups.

(2) Introduction of braces indicating the conjugation relations for maximal subgroups of types I and IIa.

(3) Rearrangement of the subgroup data: subgroups are listed according to rising index and falling space-group number within the same lattice-relation type.

(4) Analogous rearrangement of the supergroup data: the minimal supergroups are listed according to rising index and increasing space-group number. In a few cases of type-II minimal supergroups, however, the index rule is not followed.

(5) Nonconventional symbols of monoclinic subgroups: in the cases of differences between Volume A and *IT* A1 for these symbols, those used in *IT* A1 have been chosen.

(6) Isomorphic subgroups: in listing the isomorphic subgroups of lowest index (type IIc), preference was given to the index and not to the direction of the principal axis (as had been the case in previous editions of this volume).

(iii) Improvements to the data in Volume A proposed by K. Stróż:

(1) Changes of the translational part of the generators (2) and (3) of $Fd\bar{3}$ (203), origin choice 2;

(2) Changes in the geometrical description of the glide planes of type $x, 2x, z$ for the groups $R3m$ (160), $R3c$ (161), $R\bar{3}m$ (166), $R\bar{3}c$ (167), and the glide planes $\bar{x}, y, x$ for $Fm\bar{3}m$ (225), $Fd\bar{3}m$ (227);

(3) Changes in the sequence of the positions and symmetry operations for the 'rhombohedral axes' descriptions of space groups $R32$ (155), $R3m$ (160), $R3c$ (161), $R\bar{3}m$ (166) and $R\bar{3}c$ (167), *cf.* Sections 2.2.6 and 2.2.10.

The electronic preparation of the plane- and space-group tables was carried out on various Unix and Windows-based computers in Sofia, Bilbao and Karlsruhe. The development of the computer programs and the layout macros in the package file was done in parallel by different members of the team, which included Asen Kirov (Sofia), Eli Kroumova (Bilbao), Preslav Konstantinov and Mois Aroyo. Hans Wondratschek and Theo Hahn contributed to the final arrangement and checking of the data.