

Computer production of Parts 2 and 3

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The tables of this volume were produced electronically using the $\text{\LaTeX}2_{\epsilon}$ typesetting system [Lamport (1994). *A Document Preparation System*. 2nd ed. Reading: Addison-Wesley], which has the following advantages:

- (1) correcting and modifying the layout and the data are easy;
- (2) correcting or updating these for further editions of this volume should also be simple;
- (3) the cost of production for the first edition and later editions should be kept low.

A separate data file was created for every space group in each setting listed in the tables. These files contained only the information about the subgroups and supergroups, encoded using specially created $\text{\LaTeX}2_{\epsilon}$ commands and macros. These macros were defined in a separate package file which essentially contained the algorithm for the layout. Keeping the formatting information separate from the content as much as possible allowed us to change the layout by redefining the macros without changing the data files. This was done several times during the production of the tables.

The data files are relatively simple and only a minimal knowledge of $\text{\LaTeX}2_{\epsilon}$ is required to create and revise them should it be necessary later. A template file was used to facilitate the initial data entry by filling blank spaces and copying pieces of text in a text editor. It was also possible to write computer programs to extract the information from the data files directly. Such programs were used for checking the data in the files that were used to typeset the volume. The data prepared for Part 2 were later converted into a more convenient, machine-readable format so that they could be used in the database of the Bilbao Crystallographic Server at <http://www.cryst.ehu.es/>.

The final composition of all plane-group and space-group tables of maximal subgroups and minimal supergroups was done by a single computer job. References in the tables from one page to another were automatically computed. The run takes 1 to 2 minutes on a modern workstation. The result is a PostScript or pdf file which can be fed to most laser printers or other modern printing/typesetting equipment.

The resulting files were also used for the preparation of the fifth edition of *International Tables for Crystallography* Volume A (2002) (abbreviated as *IT A*). Sections of the data files of Part 2 of the present volume were transferred directly to the data files for Parts 6 and 7 of *IT A* to provide the subgroup and supergroup information listed there. The formatting macros were rewritten to achieve the layout used in *IT A*.

The different types of data in the $\text{\LaTeX}2_{\epsilon}$ files were either keyed by hand or computer-generated. The preparation of the data files of Part 2 can be summarized as follows:

- (i) Headline, origin: hand-keyed.
- (ii) Generators: hand-keyed.
- (iii) General positions: created by a program from a set of generators. The algorithm uses the well known generating process for space groups based on their solvability property, cf. Section 8.3.5 of *IT A*.
- (iv) Maximal subgroups: hand-keyed. The data for the subgroup generators (or general-position representatives for the cases of *translationengleiche* subgroups and *klassengleiche* subgroups with ‘loss of centring translations’), for transformation matrices and for conjugacy relations between subgroups were checked by specially designed computer programs.
- (v) Minimal supergroups: created automatically from the data for maximal subgroups.

The electronic preparation of the subgroup tables of Part 2 was carried out on various Unix- and Windows-based computers in Sofia, Bilbao, Stuttgart 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. Th. Hahn (Aachen) contributed to the final arrangement of the data.

The tables of Part 3 have a different layout, and a style file of their own was created for their production. Again, separate data files were prepared for every space group, containing only the information concerning the subgroups. The macros of the style file were developed by U. Müller, who also hand-keyed all files over the course of seven years.

Most of the data of Part 2 were checked using computer programs developed by F. Gähler (cf. Chapter 1.3) and A. Kirov. The relations of the Wyckoff positions (Part 3) were checked by G. Nolze (Berlin) with the aid of his computer program *POWDER CELL* [Nolze (1996). *POWDER CELL. Computer program for the calculation of X-ray powder diagrams*. Bundesanstalt für Materialforschung, Berlin]. In addition, all relations were cross-checked with the program *WYCKSPLIT* [Kroumova *et al.* (1998). *J. Appl. Cryst.* **31**, 646; <http://www.cryst.ehu.es/cryst/wpsplit.html>], with the exception of the positions of high multiplicities of some cubic space groups with subgroup indices > 50 , which could not be handled by the program.