This corresponds to an interchange of two labels and not to the more logical cyclic permutation, as used in all editions of this series. The reason for this particular transformation was to obtain short space-group symbols that indicate the setting unambiguously; thus the lattice letters were chosen as *C* (*b*-axis setting) and *B* (*c*-axis setting). The use of *A* in either case would not have distinguished between the two settings [*cf.* pp. 7, 55 and 543 of *IT* (1952); see also Table 2.1.3.12].

As a consequence of the different transformations between *b*- and *c*-axis settings in *IT* (1952) and in this volume (and all editions of this series), some space-group symbols have changed. This is apparent from a comparison of pairs such as $P12_1/c1$ & $P112_1/b$ and $C12/c1$ & $B112/b$ in *IT* (1952) with the corresponding pairs in this volume, $P12_1/c1$ & $P112_1/a$ and $C12/c1$ & $A112/a$. The symbols with *B*-centred cells appear now for cell choice 2, as can be seen from Table 2.1.3.12.

Selection of monoclinic cell. In practice, the selection of the (right-handed) unit cell of a monoclinic crystal can be approached in three ways, whereby the axes refer to the *b*-unique setting; for *c* unique similar considerations apply:

(i) Irrespective of their lengths, the basis vectors are chosen such that, in Fig. 2.1.3.12, one obtains $\mathbf{c} = \mathbf{e}$, $\mathbf{a} = \mathbf{f}$ and $\mathbf{b}$ normal to $\mathbf{a}$ and $\mathbf{c}$ pointing upwards. This corresponds to a selection of cell choice 1. It ensures that the crystal structure can always be referred directly to the description and the space-group symbol in *IT* (1935) and *IT* (1952). However, this is at the expense of possibly using a non-reduced and, in many cases, even a very awkward cell.

(ii) Selection of the reduced mesh, *i.e.* the shortest two translation vectors in the monoclinic plane are taken as axes and labelled $\mathbf{a}$ and $\mathbf{c}$, with either $a < c$ or $c < a$. This results with equal probability in one of the three cell choices described in the present volume.

(iii) Selection of the cell on special grounds, *e.g.* to compare the structure under consideration with another related crystal structure. This may result again in a non-reduced cell and it may even necessitate use of the *a*-axis setting. In all these cases, the coordinate system chosen should be carefully explained in the description of the structure.

2.1.3.16. Crystallographic groups in one dimension

In one dimension, only one crystal family, one crystal system and one Bravais lattice exist. No name or common symbol is required for any of them. All one-dimensional lattices are primitive, which is symbolized by the script letter $\mathscr{p}$; *cf.* Table 2.1.1.1.

There occur two types of one-dimensional point groups, 1 and $m \equiv \bar{1}$. The latter contains reflections through a point (reflection point or mirror point). This operation can also be described as inversion through a point, thus $m \equiv \bar{1}$ for one dimension; *cf.* Section 2.1.2.

Two types of line groups (one-dimensional space groups) exist, with Hermann–Mauguin symbols $\mathscr{p}1$ and $\mathscr{p}m \equiv \mathscr{p}\bar{1}$, which are illustrated in Fig. 2.1.3.13. Line group $\mathscr{p}1$, which consists of one-dimensional translations only, has merely one (general) position with coordinate *x*. Line group $\mathscr{p}m$ consists of one-dimensional translations and reflections through points. It has one general and two special positions. The coordinates of the general position are *x* and $\bar{x}$; the coordinate of one special position is 0, that of the other $\frac{1}{2}$. The site symmetries of both special positions are $m \equiv \bar{1}$. For $\mathscr{p}1$, the origin is arbitrary, for $\mathscr{p}m$ it is at a reflection point.

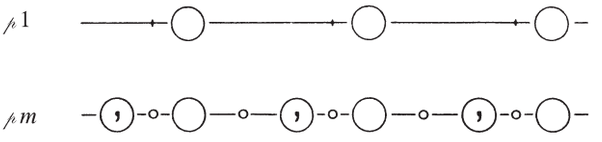

Figure 2.1.3.13
The two line groups (one-dimensional space groups). Small circles are reflection points; large circles represent the general position; in line group $\mathscr{p}1$, the vertical bars are the origins of the unit cells.

The one-dimensional *point groups* are of interest as 'edge symmetries' of two-dimensional 'edge forms'; they are listed in Table 3.2.3.1. The one-dimensional *space groups* occur as projection and section symmetries of crystal structures.

2.1.4. Computer production of the space-group tables

By P. Konstantinov and K. Momma

The space-group tables for the first (1983) edition of Volume A were produced and typeset by a computer-aided process as described by Fokkema (1983). However, the computer programs used and the data files were then lost. All corrections in the subsequent three editions were done by photocopying and 'cut-and-paste' work based on the printed version of the book.

Hence, in October 1997, a new project for the electronic production of the fifth edition of Volume A of *International Tables for Crystallography* was started. Part of this project concerned the computer generation of the plane- and space-group tables [Parts 6 and 7 of *IT* A (2002)], excluding the space-group diagrams. The aim was to be able to produce PostScript and Portable Document Format (PDF) documents that could be used for printing and displaying the tables. 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 opened the way for easy corrections and modifications of later editions and made possible the online edition of Volume A in 2006 (http://it.iucr.org/A/). Although the plane- and space-group data were encoded in a format designed for printing, they were later machine-read and transformed to other electronic formats, and were incorporated into the data files on which the Symmetry Database in the online version of *International Tables for Crystallography* (http://it.iucr.org/resources/symmetrydatabase/) and the online services offered by the Bilbao Crystallographic Server (http://www.cryst.ehu.es/) are based.

The LaTeX document preparation system (Lamport, 1994), 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. It is also worth noting the longevity of the system. Even though the hardware and operating system software used almost 20 years ago, when the project began, are now obsolete, the software is still available on all major modern computer systems. All the material – LaTeX code and data – created for the fifth edition of 2002 was re-used in the preparation of the current edition with only small changes concerning the presentation.

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. As is customary, these specially designed commands and environments are defined in a separate package

file, which essentially contains routines, called macros, that control the typographical layout of the data. Thus, the main principle of LaTeX – that of 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 running a single computer job. References in the tables from one page to another are automatically computed. The result is a PostScript file which can be fed to a laser printer or other printing or typesetting equipment. It can also be easily converted to a PDF file. It is also possible to generate the output for just one group, as accessed in the online edition, or a series of groups.

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 (*cf.* Section 1.2.2; see also Hahn & Wondratschek, 1994). The data were additionally checked by automatic comparison with the output of the computer program *SPACER* (Stróż, 1997).

Generators: transferred automatically from the data for Volume A1 of *International Tables for Crystallography* (2010), 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 (*cf.* Section 1.4.3).

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: this information appeared in the fifth revised edition of Volume A, as in the previous editions. Most of the data were automatically transferred from the data files used for the production of *IT* A1. The macros for typesetting these data were re-implemented to obtain exactly the layout of Volume A. For the current edition these data have been omitted by redefining the macros to ignore the content, which is still present in the data files.

The symmetry-element diagrams were scanned and processed in the IUCr Editorial Office in Chester.

In the first edition of *IT* A published in 1983, the general-position diagrams of the cubic groups presented in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* were replaced by small stereodiagrams. At that time, such stereodiagrams were probably the easiest way to allow three-dimensional visualization, and the same stereodiagrams were reproduced in the following editions. However, the sizes of the stereodiagrams were limited by the page size, so they were very small, and they also lacked any indication of general-position 'enantiomorph' points. The situation has changed a lot since then and three-dimensional visualization of the general positions is easily achieved with structure-drawing programs. Therefore, in this sixth edition, new general-position diagrams of the cubic groups, which are similar to those of the non-cubic groups, were created with a focus on better two-dimensional representation in print.

The new diagrams were created by K. Momma using the computer program *VESTA* (Momma & Izumi, 2011), which was extended for this purpose. The diagrams that were generated were carefully checked by comparing them with the original diagrams in the 1935 edition. The coordinates of general positions are slightly different from those used in the original diagrams and were chosen so that the general positions overlap as little as possible in the two-dimensional orthogonal projection of the diagrams. The coordinates of general positions used are:

(i) 0.0375, 0.1125, 0.098 for space-group Nos. 198, 199, 205, 206, 212, 213, 214, 220 and 230;
(ii) 0.065, 0.12, 0.048 for the second diagrams of space-group Nos. 212, 214 and 230;
(iii) 0.435, 0.38, 0.452 for the second diagram of space-group No. 213;
(iv) 0.31, 0.095, 0.21 for the second diagram of space-group No. 220; and
(v) $0.048x$, $0.12y$, $0.089z$ for the remaining space groups, where x, y, z is the first coordinate triplet of the highest symmetry Wyckoff position of the space group.

In addition, three-dimensional-style tilted general-position diagrams were created by *VESTA* for each of the ten space groups of the $m\bar{3}m$ crystal class. These diagrams can be reproduced and visualized in three dimensions using *VESTA*. They were provided in the form of Portable Network Graphics (PNG) raster images and were included in the page layout of the space-group tables with some scaling and cropping.

The preparation of the plane- and space-group tables was carried out on various computer platforms in Sofia, Bilbao, Karlsruhe, Tsukuba and Chester. The development of the computer programs and the layout macros in the LaTeX package file, and the preparation of the diagrams were done in parallel by different members of the team, which included Asen Kirov (Sofia), Eli Kroumova (Bilbao), Koichi Momma, Preslav Konstantinov and Mois Aroyo, and staff at the Editorial Office in Chester.

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