2. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

glide planes (*e* before *a* before *b* before *c* before *n*) is *not* followed. Instead, in order to bring out the relations between the various settings and cell choices, the glide-plane symbol always refers to that glide plane which intersects the conventional origin.

Example: No. 15, standard short symbol *C*2/*c*

The full symbols for the three cell choices (rows) and the three unique axes (columns) read

$$C12/c1 \quad A12/n1 \quad I12/a1$$
$$A112/a \quad B112/n \quad I112/b$$
$$B2/b11 \quad C2/n11 \quad I2/c11.$$

Application of the priority rule would have resulted in the following symbols

$$C12/c1 \quad A12/a1 \quad I12/a1$$
$$A112/a \quad B112/b \quad I112/a$$
$$B2/b11 \quad C2/c11 \quad I2/b11.$$

Here, the transformation properties are obscured.

2.2.16.4. *Comparison with earlier editions of International Tables*

In *IT* (1935), each monoclinic space group was presented in one description only, with *b* as the unique axis. Hence, only one short Hermann–Mauguin symbol was needed.

In *IT* (1952), the *c*-axis setting (first setting) was newly introduced, in addition to the *b*-axis setting (second setting). This extension was based on a decision of the Stockholm General Assembly of the International Union of Crystallography in 1951 [*cf. Acta Cryst.* (1951), **4**, 569 and *Preface* to *IT* (1952)]. According to this decision, the *b*-axis setting should continue to be accepted as standard for morphological and structural studies. The two settings led to the introduction of *full* Hermann–Mauguin symbols for *all* 13 monoclinic space groups (*e.g.* $P12_1/c1$ and $P112_1/b$) and of two different *standard short* symbols (*e.g.* $P2_1/c$ and $P2_1/b$) for the *eight* space groups with centred lattices or glide planes [*cf.* p. 545 of *IT* (1952)]. In the present volume, only one of these standard short symbols is retained (see above and Section 2.2.3).

The *c*-axis setting (primed labels) was obtained from the *b*-axis setting (unprimed labels) by the following transformation

$$(\mathbf{a'b'\underline{c}'}) = (\mathbf{a\underline{b}c}) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix} = (\mathbf{ac\underline{b}}).$$

This corresponds to an interchange of two labels and not to the more logical cyclic permutation, as used in the present volume. 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 2.2.16.2].

As a consequence of the different transformations between *b*- and *c*-axis settings in *IT* (1952) and in this volume, 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 2.2.16.2.
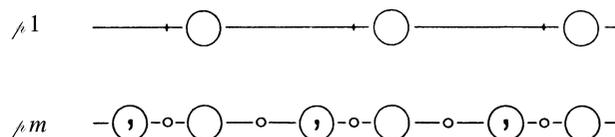

Fig. 2.2.17.1. The two line groups (one-dimensional space groups). Small circles are reflection points; large circles represent the general position; in line group $\rho 1$, the vertical bars are the origins of the unit cells.

2.2.16.5. *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. 2.2.16.1, 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.

2.2.17. 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 ρ; *cf.* Chapter 1.2.

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.* Chapters 1.3 and 1.4.

Two types of line groups (one-dimensional space groups) exist, with Hermann–Mauguin symbols $\rho 1$ and $\rho m \equiv \rho\bar{1}$, which are illustrated in Fig. 2.2.17.1. Line group $\rho 1$, which consists of one-dimensional translations only, has merely one (general) position with coordinate *x*. Line group ρm 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 $\rho 1$, the origin is arbitrary, for ρm it is at a reflection point.

The one-dimensional *point groups* are of interest as 'edge symmetries' of two-dimensional 'edge forms'; they are listed in Table 10.1.2.1. The one-dimensional *space groups* occur as projection and section symmetries of crystal structures.

references