## 2.2. CONTENTS AND ARRANGEMENT OF THE TABLES

Table 2.2.16.1 lists the setting symbols for the six monoclinic settings in three equivalent forms, starting with the symbols **a** $\underline{\mathbf{b}}$ **c** (first line), **a b** $\underline{\mathbf{c}}$ (second line) and $\underline{\mathbf{a}}$ **b c** (third line); the unique axis is underlined. These symbols are also found in the headline of the synoptic Table 4.3.2.1, which lists the space-group symbols for all monoclinic settings and cell choices. Again, the corresponding transformation matrices are listed in Table 5.1.3.1.

In the space-group tables, only the settings with *b* and *c* unique are treated and for these only the left-hand members of the double entries in Table 2.2.16.1. This implies, for instance, that the *c*-axis setting is obtained from the *b*-axis setting by cyclic permutation of the labels, *i.e.* by the transformation

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

In the present discussion, also the setting with *a* unique is included, as this setting occurs in the subgroup entries of Part 7 and in Table 4.3.2.1. The *a*-axis setting $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{c}}\mathbf{a}\mathbf{b}$ is obtained from the *c*-axis setting also by cyclic permutation of the labels and from the *b*-axis setting by the reverse cyclic permutation: $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{b}}\mathbf{c}\mathbf{a}$.

By the conventions described above, the setting of each of the cell choices 1, 2 and 3 is determined once the label and the direction of the unique-axis vector have been selected. Six of the nine resulting possibilities are illustrated in Fig. 2.2.6.4.

### 2.2.16.3. *Cell choices and settings in the present tables*

There are five monoclinic space groups for which the Hermann–Mauguin symbols are independent of the cell choice, *viz* those space groups that do *not* contain centred lattices or glide planes:

$P2$ (No. 3), $P2_1$ (4), $Pm$ (6), $P2/m$ (10), $P2_1/m$ (11).

In these cases, description of the space group by one cell choice is sufficient.

For the eight monoclinic space groups *with centred lattices or glide planes*, the Hermann–Mauguin symbol depends on the choice of the oblique axes with respect to the glide vector and/or the centring vector. These eight space groups are:

$C2$ (5), $Pc$ (7), $Cm$ (8), $Cc$ (9), $C2/m$ (12), $P2/c$ (13), $P2_1/c$ (14), $C2/c$ (15).

Here, the glide vector or the projection of the centring vector onto the monoclinic plane are always directed along *one* of the vectors **e**, **f** or **g** in Fig. 2.2.16.1, *i.e.* are parallel to the shortest, the second-shortest or the third-shortest translation vector in the monoclinic plane (note that a glide vector and the projection of a centring vector cannot be parallel). This results in three possible orientations of the glide vector or the centring vector with respect to these crystal axes, and thus in three different full Hermann–Mauguin symbols (*cf.* Section 2.2.4) for each setting of a space group.

Table 2.2.16.2 lists the symbols for centring types and glide planes for the cell choices 1, 2, 3. The order of the three cell choices is defined as follows: The symbols occurring in the familiar 'standard short monoclinic space-group symbols' (see Section 2.2.3) define cell choice 1; for 'unique axis *b*', this applies to the centring type *C* and the glide plane *c*, as in $Cm$ (8) and $P2_1/c$ (14). Cell choices 2 and 3 follow from the anticlockwise order 1–2–3 in Fig. 2.2.6.4 and their space-group symbols can be obtained from Table 2.2.16.2. The *c*-axis and the *a*-axis settings then are derived from the *b*-axis setting by cyclic permutations of the axial labels, as described in Section 2.2.16.2.

In the two space groups $Cc$ (9) and $C2/c$ (15), glide planes occur in pairs, *i.e.* each vector **e**, **f**, **g** is associated either with a glide vector or with the centring vector of the cell. For $Pc$ (7), $P2/c$ (13) and $P2_1/c$ (14), which contain only one type of glide plane, the left-hand member of each pair of glide planes in Table 2.2.16.2 applies.

Table 2.2.16.1. *Monoclinic setting symbols (unique axis is underlined)*

| Unique axis *b* | | Unique axis *c* | | Unique axis *a* | | |
|---|---|---|---|---|---|---|
| **a**$\underline{\mathbf{b}}$**c** | **c**$\bar{\underline{\mathbf{b}}}$**a** | **ca**$\underline{\mathbf{b}}$ | **ac**$\bar{\underline{\mathbf{b}}}$ | **b**$\underline{\mathbf{c}}$**a** | **b**$\bar{\underline{\mathbf{c}}}$**a** | Starting set **a**$\underline{\mathbf{b}}$**c** |
| **bc**$\underline{\mathbf{a}}$ | **ac**$\bar{\underline{\mathbf{b}}}$ | **a**$\underline{\mathbf{b}}$**c** | **ba**$\bar{\underline{\mathbf{c}}}$ | **c**$\underline{\mathbf{a}}$**b** | **c**$\bar{\underline{\mathbf{a}}}$**b** | Starting set **a**$\underline{\mathbf{b}}$**c** |
| **ca**$\underline{\mathbf{b}}$ | **ba**$\bar{\underline{\mathbf{c}}}$ | **bc**$\underline{\mathbf{a}}$ | **cb**$\bar{\underline{\mathbf{a}}}$ | **a**$\underline{\mathbf{b}}$**c** | **a**$\bar{\underline{\mathbf{c}}}$**b** | Starting set **a**$\underline{\mathbf{b}}$**c** |

*Note*: An interchange of two axes involves a change of the handedness of the coordinate system. In order to keep the system right-handed, one sign reversal is necessary.

Table 2.2.16.2. *Symbols for centring types and glide planes of monoclinic space groups*

| Setting | | Cell choice | | |
|---|---|---|---|---|
| | | 1 | 2 | 3 |
| Unique axis *b* | Centring type | *C* | *A* | *I* |
| | Glide planes | *c*, *n* | *n*, *a* | *a*, *c* |
| Unique axis *c* | Centring type | *A* | *B* | *I* |
| | Glide planes | *a*, *n* | *n*, *b* | *b*, *a* |
| Unique axis *a* | Centring type | *B* | *C* | *I* |
| | Glide planes | *b*, *n* | *n*, *c* | *c*, *b* |

In the space-group tables of this volume, the following treatments of monoclinic space groups are given:

(1) *Two complete descriptions* for each of the five monoclinic space groups with primitive lattices and without glide planes, one for 'unique axis *b*' and one for 'unique axis *c*', similar to the treatment in *IT* (1952).

(2) A total of *six descriptions* for each of the eight space groups with centred lattices or glide planes, as follows:

(*a*) *One complete* description for 'unique axis *b*' and 'cell choice' 1. This is considered the standard description of the space group, and its *short* Hermann–Mauguin symbol is used as the *standard* symbol of the space group.

This standard short symbol corresponds to the one symbol of *IT* (1935) and to that of the *b*-axis setting in *IT* (1952), *e.g.* $P2_1/c$ or $C2/c$. It serves only to identify the space-group type but carries no information about the setting or cell choice of a particular description. The *standard short symbol* is given in the headline of every description of a monoclinic space group; *cf.* Section 2.2.3.

(*b*) *Three condensed* (synoptic) descriptions for 'unique axis *b*' and the three 'cell choices' 1, 2, 3. Cell choice 1 is repeated to facilitate comparison with the other cell choices. Diagrams are provided to illustrate the three cell choices: *cf.* Section 2.2.6.

(*c*) *One complete* description for 'unique axis *c*' and 'cell choice' 1.

(*d*) *Three condensed* (synoptic) descriptions for 'unique axis *c*' and the three 'cell choices' 1, 2, 3. Again cell choice 1 is repeated and appropriate diagrams are provided.

All settings and cell choices are identified by the appropriate *full* Hermann–Mauguin symbols (*cf.* Section 2.2.4), *e.g.* $C12/c1$ or $I112/b$. For the two space groups $Cc$ (9) and $C2/c$ (15) with pairs of different glide planes, the 'priority rule' (*cf.* Section 4.1.1) for





references