Under *supergroups* **II** of $Pna2_1$ (33), the corresponding entry reads [2] $Pba2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (32); thus $\mathbf{c}(Pba2) = \frac{1}{2}\mathbf{c}(Pna2_1)$.

(2) Tetragonal *k* space groups with *P* cells. For index [2], the relations between the *conventional* basis vectors of the group and the subgroup read (*cf.* Fig. 5.1.3.5)

$\mathbf{a}' = \mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$ ($\mathbf{a}', \mathbf{b}'$ for the subgroup).

Thus, the basis vectors of the supergroup are

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} - \mathbf{b})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ ($\mathbf{a}', \mathbf{b}'$ for the supergroup).

An alternative description is

$\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$ ($\mathbf{a}', \mathbf{b}'$ for the subgroup)

$\mathbf{a}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ ($\mathbf{a}', \mathbf{b}'$ for the supergroup).

(3) Hexagonal *k* space groups. For index [3], the relations between the *conventional* basis vectors of the sub- and supergroup read (*cf.* Fig 5.1.3.8)

$\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + 2\mathbf{b}$ ($\mathbf{a}', \mathbf{b}'$ for the subgroup).

Thus, the basis vectors of the supergroup are

$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b})$ ($\mathbf{a}', \mathbf{b}'$ for the supergroup).

An alternative description is

$\mathbf{a}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$ ($\mathbf{a}', \mathbf{b}'$ for the subgroup)

$\mathbf{a}' = \frac{1}{3}(\mathbf{a} - \mathbf{b})$, $\mathbf{b}' = \frac{1}{3}(\mathbf{a} + 2\mathbf{b})$ ($\mathbf{a}', \mathbf{b}'$ for the supergroup).

2.2.16. Monoclinic space groups

In this volume, space groups are described by one (or at most two) conventional coordinate systems (*cf.* Sections 2.1.3 and 2.2.2). Eight monoclinic space groups, however, are treated more extensively. In order to provide descriptions for frequently encountered cases, they are given in six versions.

The description of a monoclinic crystal structure in this volume, including its Hermann–Mauguin space-group symbol, depends upon two choices:

(i) the unit cell chosen, here called 'cell choice';

(ii) the labelling of the edges of this cell, especially of the monoclinic symmetry direction ('unique axis'), here called 'setting'.

2.2.16.1. *Cell choices*

One edge of the cell, *i.e.* one crystal axis, is always chosen along the monoclinic symmetry direction. The other two edges are located in the plane perpendicular to this direction and coincide with translation vectors in this 'monoclinic plane'. It is sensible and common practice (see below) to choose these two basis vectors from the *shortest three* translation vectors in that plane. They are shown in Fig. 2.2.16.1 and labelled **e**, **f** and **g**, in order of increasing length.* The two shorter vectors span the 'reduced mesh', here **e** and **f**; for this mesh, the monoclinic angle is $\leq 120°$, whereas for the other two primitive meshes larger angles are possible.

Other choices of the basis vectors in the monoclinic plane are possible, provided they span a primitive mesh. It turns out, however, that the space-group symbol for any of these (non-reduced) meshes already occurs among the symbols for the three meshes formed by **e**, **f**, **g** in Fig. 2.2.16.1; hence only these cases need be considered. They are designated in this volume as 'cell choice 1, 2 or 3' and are depicted in Fig. 2.2.6.4. The transformation matrices for the three cell choices are listed in Table 5.1.3.1.

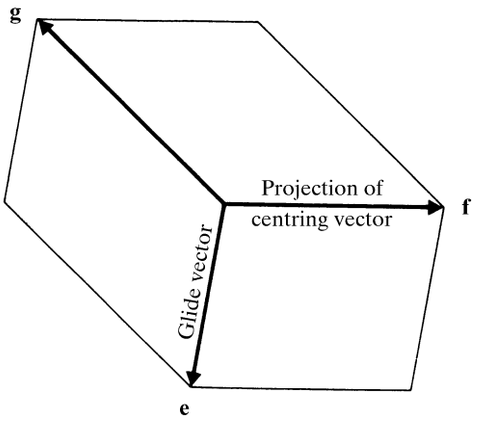

Fig. 2.2.16.1. The three primitive two-dimensional cells which are spanned by the shortest three translation vectors **e**, **f**, **g** in the monoclinic plane. For the present discussion, the glide vector is considered to be along **e** and the projection of the centring vector along **f**.

2.2.16.2. *Settings*

The term *setting* of a cell or of a space group refers to the assignment of labels (*a*, *b*, *c*) and directions to the edges of a given unit cell, resulting in a set of basis vectors **a**, **b**, **c**. (For orthorhombic space groups, the six settings are described and illustrated in Section 2.2.6.4.)

The symbol for each setting is a shorthand notation for the transformation of a given starting set **abc** into the setting considered. It is called here 'setting symbol'. For instance, the setting symbol **bca** stands for

$$\mathbf{a}' = \mathbf{b}, \quad \mathbf{b}' = \mathbf{c}, \quad \mathbf{c}' = \mathbf{a}$$

or

$$(\mathbf{a}'\mathbf{b}'\mathbf{c}') = (\mathbf{abc})\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = (\mathbf{bca}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. (Note that the setting symbol **bca** does *not* mean that the old vector **a** changes its label to **b**, the old vector **b** changes to **c**, and the old **c** changes to **a**.) Transformation of one setting into another preserves the shape of the cell and its orientation relative to the lattice. The matrices of these transformations have *one* entry $+1$ or -1 in each row and column; all other entries are 0.

In monoclinic space groups, one axis, the monoclinic symmetry direction, is unique. Its label must be chosen first and, depending upon this choice, one speaks of 'unique axis *b*', 'unique axis *c*' or 'unique axis *a*'.† Conventionally, the positive directions of the two further ('oblique') axes are oriented so as to make the monoclinic angle non-acute, *i.e.* $\geq 90°$, and the coordinate system right-handed. For the three cell choices, settings obeying this condition and having the same label and direction of the unique axis are considered as one setting; this is illustrated in Fig. 2.2.6.4.

Note: These three cases of labelling the monoclinic axis are often called somewhat loosely *b*-axis, *c*-axis and *a*-axis 'settings'. It must be realized, however, that the choice of the 'unique axis' alone does *not* define a *single* setting but only a *pair*, as for each cell the labels of the two oblique axes can be interchanged.

* These three vectors obey the 'closed-triangle' condition $\mathbf{e} + \mathbf{f} + \mathbf{g} = \mathbf{0}$; they can be considered as two-dimensional homogeneous axes.

† In *IT* (1952), the terms '1st setting' and '2nd setting' were used for 'unique axis *c*' and 'unique axis *b*'. In the present volume, these terms have been dropped in favour of the latter names, which are unambiguous.

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.

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**
bca	**a**$\bar{\underline{\mathbf{c}}}$**b**	**a**$\underline{\mathbf{b}}$**c**	**ba**$\bar{\underline{\mathbf{c}}}$	**c**$\underline{\mathbf{a}}$**b**	**c**$\bar{\underline{\mathbf{a}}}$**ba**	Starting set **a**$\underline{\mathbf{b}}$**c**
c$\underline{\mathbf{a}}$**b**	**b**$\bar{\underline{\mathbf{a}}}$**c**	**bc**$\underline{\mathbf{a}}$	**cb**$\bar{\underline{\mathbf{a}}}$	$\underline{\mathbf{a}}$**bc**	$\bar{\underline{\mathbf{a}}}$**cb**	Starting set $\underline{\mathbf{a}}$**bc**

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*

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:

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

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:

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

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.

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

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 $C2/c$

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

$$\begin{array}{lll} C12/c1 & A12/n1 & I12/a1 \\ A112/a & B112/n & I112/b \\ B2/b11 & C2/n11 & I2/c11. \end{array}$$

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

$$\begin{array}{lll} C12/c1 & A12/a1 & I12/a1 \\ A112/a & B112/b & I112/a \\ B2/b11 & C2/c11 & I2/b11. \end{array}$$

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

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

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.

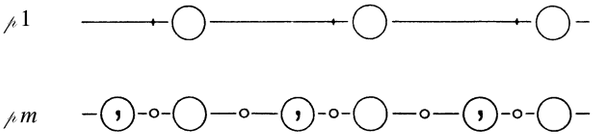

Fig. 2.2.17.1. The two line groups (one-dimensional space groups). Small circles are reflection points; large circles represent the general position; in line group $\not p1$, the vertical bars are the origins of the unit cells.

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 $\not p$; *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 $\not p1$ and $\not pm \equiv \not p\bar{1}$, which are illustrated in Fig. 2.2.17.1. Line group $\not p1$, which consists of one-dimensional translations only, has merely one (general) position with coordinate x. Line group $\not pm$ 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 $\not p1$, the origin is arbitrary, for $\not pm$ 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.