

## 2.2. CONTENTS AND ARRANGEMENT OF THE TABLES

same or of the enantiomorphic space-group type as  $\mathcal{G}$ . The kind of listing is the same as for block **IIb**. Again, one entry may correspond to more than one isomorphic subgroup.

As the number of maximal isomorphic subgroups of a space group is always infinite, the data in block **IIc** are restricted to the subgroups of lowest index. Different kinds of cell enlargements are presented. For monoclinic, tetragonal, trigonal and hexagonal space groups, cell enlargements both parallel and perpendicular to the main rotation axis are listed; for orthorhombic space groups, this is the case for all three directions,  $a$ ,  $b$  and  $c$ . Two isomorphic subgroups  $\mathcal{H}_1$  and  $\mathcal{H}_2$  of equal index but with cell enlargements in different directions may, nevertheless, play an analogous role with respect to  $\mathcal{G}$ . In terms of group theory,  $\mathcal{H}_1$  and  $\mathcal{H}_2$  then are conjugate subgroups in the affine normalizer of  $\mathcal{G}$ , *i.e.* they are mapped onto each other by automorphisms of  $\mathcal{G}$ .<sup>\*</sup> Such subgroups are collected into one entry, with the different vector relationships separated by ‘or’ and placed within one pair of parentheses; *cf.* example (4).

*Examples*

(1)  $\mathcal{G}$ :  $P\bar{3}1c$  (163)

**IIc** [3]  $P\bar{3}1c$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (163); [4]  $P\bar{3}1c$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) (163).

The first subgroup of index [3] entails an enlargement of the  $c$  axis, the second one of index [4] an enlargement of the mesh size in the  $a, b$  plane.

(2)  $\mathcal{G}$ :  $P23$  (195)

**IIc** [27]  $P23$  ( $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$ ) (195).

It seems surprising that [27] is the lowest index listed, even though another isomorphic subgroup of index [8] exists. The latter subgroup, however, is not maximal, as chains of maximal non-isomorphic subgroups can be constructed as follows:

$P23 \rightarrow [4] I23$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$ )  $\rightarrow [2] P23$  ( $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ )

or

$P23 \rightarrow [2] F23$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$ )  $\rightarrow [4] P23$  ( $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ ).

(3)  $\mathcal{G}$ :  $P3_112$  (151)

**IIc** [2]  $P3_112$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (153); [4]  $P3_112$  ( $\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$ ) (151);  
[7]  $P3_112$  ( $\mathbf{c}' = 7\mathbf{c}$ ) (151).

Note that the isomorphic subgroup of index [4] with  $\mathbf{c}' = 4\mathbf{c}$  is not listed, because it is not maximal. This is apparent from the chain

$P3_112 \rightarrow [2] P3_112$  ( $\mathbf{c}' = 2\mathbf{c}$ )  $\rightarrow [2] P3_112$  ( $\mathbf{c}'' = 2\mathbf{c}' = 4\mathbf{c}$ ).

(4)  $\mathcal{G}_1$ :  $Pnmm$  (58)

**IIc** [3]  $Pnmm$  ( $\mathbf{a}' = 3\mathbf{a}$  or  $\mathbf{b}' = 3\mathbf{b}$ ) (58); [3]  $Pnmm$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (58);  
but  $\mathcal{G}_2$ :  $Pnna$  (52)

**IIc** [3]  $Pnna$  ( $\mathbf{a}' = 3\mathbf{a}$ ) (52); [3]  $Pnna$  ( $\mathbf{b}' = 3\mathbf{b}$ ) (52);  
[3]  $Pnna$  ( $\mathbf{c}' = 3\mathbf{c}$ ) (52).

For  $\mathcal{G}_1 = Pnmm$ , the  $x$  and  $y$  directions are analogous, *i.e.* they may be interchanged by automorphisms of  $\mathcal{G}_1$ . Such an automorphism does not exist for  $\mathcal{G}_2 = Pnna$  because this space group contains glide reflections  $a$  but not  $b$ .

## 2.2.15.3. Minimal non-isomorphic supergroups

If  $\mathcal{G}$  is a maximal subgroup of a group  $\mathcal{S}$ , then  $\mathcal{S}$  is called a minimal supergroup of  $\mathcal{G}$ . Minimal non-isomorphic supergroups are

again subdivided into two types, the *translationengleiche* or  $t$  supergroups **I** and the *klassengleiche* or  $k$  supergroups **II**. For the minimal  $t$  supergroups **I** of  $\mathcal{G}$ , the listing contains the index [ $i$ ] of  $\mathcal{G}$  in  $\mathcal{S}$ , the *conventional* Hermann–Mauguin symbol of  $\mathcal{S}$  and its space-group number in parentheses.

There are two types of minimal  $k$  supergroups **II**: supergroups with additional centring translations (which would correspond to the **IIa** type) and supergroups with smaller conventional unit cells than that of  $\mathcal{G}$  (type **IIb**). Although the subdivision between **IIa** and **IIb** supergroups is not indicated in the tables, the list of minimal supergroups with additional centring translations (**IIa**) always precedes the list of **IIb** supergroups. The information given is similar to that for the non-isomorphic subgroups **IIb**, *i.e.*, where applicable, the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of  $\mathcal{S}$  and its space-group number. The supergroups are listed in order of increasing index and increasing space-group number.

The block of supergroups contains only the *types* of the non-isomorphic minimal supergroups  $\mathcal{S}$  of  $\mathcal{G}$ , *i.e.* each entry may correspond to more than one supergroup  $\mathcal{S}$ . In fact, the list of minimal supergroups  $\mathcal{S}$  of  $\mathcal{G}$  should be considered as a backwards reference to those space groups  $\mathcal{S}$  for which  $\mathcal{G}$  appears as a maximal subgroup. Thus, the relation between  $\mathcal{S}$  and  $\mathcal{G}$  can be found in the subgroup entries of  $\mathcal{S}$ .

*Example:*  $\mathcal{G}$ :  $Pna2_1$  (33)

Minimal non-isomorphic supergroups

**I** [2]  $Pnna$  (52); [2]  $Pccn$  (56); [2]  $Pbcn$  (60); [2]  $Pnma$  (62).

**II** ... [2]  $Pnm2_1$  ( $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ ) ( $Pmn2_1, 31$ ); ...

Block **I** lists, among others, the entry [2]  $Pnma$  (62). Looking up the *subgroup* data of  $Pnma$  (62), one finds in block **I** the entry [2]  $Pn2_1a$  ( $Pna2_1$ ). This shows that the setting of  $Pnma$  does not correspond to that of  $Pna2_1$  but rather to that of  $Pn2_1a$ . To obtain the supergroup  $\mathcal{S}$  referred to the basis of  $Pna2_1$ , the basis vectors  $\mathbf{b}$  and  $\mathbf{c}$  must be interchanged. This changes  $Pnma$  to  $Pnam$ , which is the correct symbol of the supergroup of  $Pna2_1$ .

*Note on R supergroups of trigonal P space groups:* The trigonal  $P$  space groups Nos. 143–145, 147, 150, 152, 154, 156, 158, 164 and 165 each have two rhombohedral supergroups of type **II**. They are distinguished by different additional centring translations which correspond to the ‘obverse’ and ‘reverse’ settings of a triple hexagonal  $R$  cell; *cf.* Chapter 1.2. In the supergroup tables of Part 7, these cases are described as [3]  $R3$  (obverse) (146); [3]  $R3$  (reverse) (146) *etc.*

## 2.2.15.4. Minimal isomorphic supergroups of lowest index

No data are listed for isomorphic supergroups **IIc** because they can be derived directly from the corresponding data of *subgroups* **IIc** (*cf.* Part 13).

## 2.2.15.5. Note on basis vectors

In the *subgroup* data,  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$  are the basis vectors of the subgroup  $\mathcal{H}$  of the space group  $\mathcal{G}$ . The latter has the basis vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ . In the *supergroup* data,  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$  are the basis vectors of the supergroup  $\mathcal{S}$  and  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  are again the basis vectors of  $\mathcal{G}$ . Thus,  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  and  $\mathbf{a}'$ ,  $\mathbf{b}'$ ,  $\mathbf{c}'$  exchange their roles if one considers the same group–subgroup relation in the subgroup and the supergroup tables.

*Examples*

(1)  $\mathcal{G}$ :  $Pba2$  (32)

Listed under *subgroups* **IIb**, one finds, among other entries, [2]  $Pna2_1$  ( $\mathbf{c}' = 2\mathbf{c}$ ) (33); thus,  $\mathbf{c}(Pna2_1) = 2\mathbf{c}(Pba2)$ .

<sup>\*</sup> For normalizers of space groups, see Section 8.3.6 and Part 15, where also references to automorphisms are given.

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

Under *supergroups*  $\Pi$  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)

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

Thus, the basis vectors of the supergroup are

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

An alternative description is

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

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

- (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)

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

Thus, the basis vectors of the supergroup are

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

An alternative description is

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

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

### 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  $\mathbf{e}$ ,  $\mathbf{f}$  and  $\mathbf{g}$ , in order of increasing length.\* The two shorter vectors span the ‘reduced mesh’, here  $\mathbf{e}$  and  $\mathbf{f}$ ; for this mesh, the monoclinic angle is  $\leq 120^\circ$ , 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  $\mathbf{e}$ ,  $\mathbf{f}$ ,  $\mathbf{g}$  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.

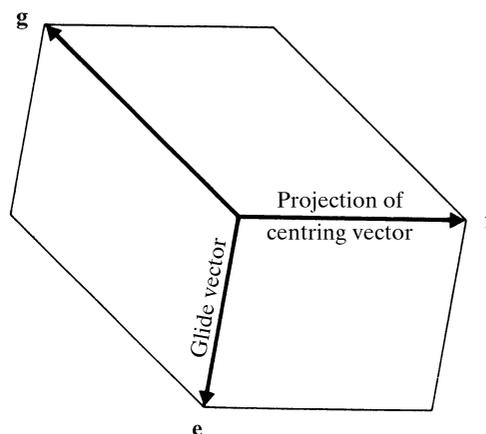


Fig. 2.2.16.1. The three primitive two-dimensional cells which are spanned by the shortest three translation vectors  $\mathbf{e}$ ,  $\mathbf{f}$ ,  $\mathbf{g}$  in the monoclinic plane. For the present discussion, the glide vector is considered to be along  $\mathbf{e}$  and the projection of the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

#### 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  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ . (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  $\mathbf{abc}$  into the setting considered. It is called here ‘setting symbol’. For instance, the setting symbol  $\mathbf{bca}$  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  $\mathbf{bca}$  does *not* mean that the old vector  $\mathbf{a}$  changes its label to  $\mathbf{b}$ , the old vector  $\mathbf{b}$  changes to  $\mathbf{c}$ , and the old  $\mathbf{c}$  changes to  $\mathbf{a}$ .) 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.*  $\geq 90^\circ$ , 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.