International Tables for Crystallography (2006). Vol. A, Section 2.2.15, pp. 35–38.

is equal to the glide vector of the glide plane. Thus, a reduction of the translation period in that particular direction takes place.

(iv) Reflection planes *parallel* to the projection direction project as reflection lines. Glide planes project as glide lines or as reflection lines, depending upon whether the glide vector has or has not a component parallel to the projection plane.

(v) Centres of symmetry, as well as $\bar{3}$ axes in *arbitrary* orientation, project as twofold rotation points.

Example: $C12/c1$ (15, *b* unique, cell choice 1)

The *C*-centred cell has lattice points at 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0$. In all projections, the centre $\bar{1}$ projects as a twofold rotation point.

Projection along [001]: The plane cell is centred; $2 \parallel [010]$ projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* vanishes and thus *c* projects as *m*.

Result: Plane group *c2mm* (9), $\mathbf{a}' = \mathbf{a}_p, \mathbf{b}' = \mathbf{b}$.

Projection along [100]: The periodicity along *b* is halved because of the *C* centring; $2 \parallel [010]$ projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* is retained and thus *c* projects as *g*.

Result: Plane group *p2gm* (7), $\mathbf{a}' = \mathbf{b}/2,\ \mathbf{b}' = \mathbf{c}_p$.

Projection along [010]: The periodicity along *a* is halved because of the *C* centring; that along *c* is halved owing to the glide component $(0, 0, \frac{1}{2})$ of glide plane *c*; $2 \parallel [010]$ projects as 2.

Result: Plane group *p*2 (2), $\mathbf{a}' = \mathbf{c}/2, \mathbf{b}' = \mathbf{a}/2$.

Further details about the geometry of projections can be found in publications by Buerger (1965) and Biedl (1966).

2.2.15. Maximal subgroups and minimal supergroups

The present section gives a brief summary, without theoretical explanations, of the sub- and supergroup data in the space-group tables. The theoretical background is provided in Section 8.3.3 and Part 13. Detailed sub- and supergroup data are given in *International Tables for Crystallography* Volume A1 (2004).

2.2.15.1. *Maximal non-isomorphic subgroups**

The maximal non-isomorphic subgroups $\mathcal{H}$ of a space group $\mathcal{G}$ are divided into two types:

I	*translationengleiche*	or *t* subgroups
II	*klassengleiche*	or *k* subgroups.

For practical reasons, type **II** is subdivided again into two blocks:

IIa the conventional cells of $\mathcal{G}$ and $\mathcal{H}$ are the same

IIb the conventional cell of $\mathcal{H}$ is larger than that of $\mathcal{G}$. †

Block **IIa** has no entries for space groups $\mathcal{G}$ with a primitive cell. For space groups $\mathcal{G}$ with a centred cell, it contains those maximal subgroups $\mathcal{H}$ that have lost some or all centring translations of $\mathcal{G}$ but none of the integral translations ('decentring' of a centred cell).

Within each block, the subgroups are listed in order of increasing index [*i*] and in order of decreasing space-group number for each value of *i*.

(i) *Blocks* **I** *and* **IIa**

In blocks **I** and **IIa**, *every* maximal subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is listed with the following information:

[*i*] HMS1 (HMS2, No.) Sequence of numbers.

The symbols have the following meaning:

[*i*]: index of $\mathcal{H}$ in $\mathcal{G}$ (*cf.* Section 8.1.6, footnote);

HMS1: Hermann–Mauguin symbol of $\mathcal{H}$, referred to the coordinate system and setting of $\mathcal{G}$; this symbol may be unconventional;

(HMS2, No.): conventional short Hermann–Mauguin symbol of $\mathcal{H}$, given only if HMS1 is not in conventional short form, and the space-group number of $\mathcal{H}$.

Sequence of numbers: coordinate triplets of $\mathcal{G}$ retained in $\mathcal{H}$. The numbers refer to the numbering scheme of the coordinate triplets of the general position of $\mathcal{G}$ (*cf.* Section 2.2.9). The following abbreviations are used:

Block **I** (all translations retained):

Number +	Coordinate triplet given by *Number*, plus those obtained by adding all centring translations of $\mathcal{G}$.
(*Numbers*) +	The same, but applied to all *Numbers* between parentheses.

Block **IIa** (not all translations retained):

Number + (t_1, t_2, t_3)	Coordinate triplet obtained by adding the translation t_1, t_2, t_3 to the triplet given by *Number*.
(*Numbers*) + (t_1, t_2, t_3)	The same, but applied to all *Numbers* between parentheses.

In blocks **I** and **IIa**, sets of conjugate subgroups are linked by left-hand braces. For an example, see space group $R\bar{3}$ (148) below.

Examples

(1) $\mathcal{G}$: $C1m1$ (8)

I	[2] $C1$ $(P1, 1)$	1+
IIa	[2] $P1a1$ $(Pc, 7)$	1; 2 + (1/2, 1/2, 0)
	[2] $P1m1$ $(Pm, 6)$	1; 2

where the numbers have the following meaning:

1+	$x, y, z;$	$x + 1/2, y + 1/2, z$
1; 2	$x, y, z;$	$x, \bar{y}, z$
1; 2 + (1/2, 1/2, 0)	$x, y, z;$	$x + 1/2, \bar{y} + 1/2, z.$

(2) $\mathcal{G}$: $Fdd2$ (43)

I [2] $F112$ $(C2, 5)$ (1; 2)+

where the numbers have the following meaning:

(1; 2)+ $x, y, z;$ $x + 1/2, y + 1/2, z;$
$x + 1/2, y, z + 1/2;$ $x, y + 1/2, z + 1/2;$
$\bar{x}, \bar{y}, z;$ $\bar{x} + 1/2, \bar{y} + 1/2, z;$
$\bar{x} + 1/2, \bar{y}, z + 1/2;$ $\bar{x}, \bar{y} + 1/2, z + 1/2.$

(3) $\mathcal{G}$: $P4_2/nmc = P4_2/n2_1/m2/c$ (137)

I [2] $P2/n2_1/m1$ $(Pmmn, 59)$ 1; 2; 5; 6; 9; 10; 13; 14.

Operations $4_2, 2$ and *c*, occurring in the Hermann–Mauguin symbol of $\mathcal{G}$, are lacking in $\mathcal{H}$. In the unconventional 'tetragonal version' $P2/n2_1/m1$ of the symbol of $\mathcal{H}$, $2_1/m$ stands for two sets of $2_1/m$ (along the two orthogonal secondary symmetry directions), implying that $\mathcal{H}$ is orthorhombic. In the conventional 'orthorhombic version', the full symbol of $\mathcal{H}$ reads $P2_1/m2_1/m2/n$ and the short symbol *Pmmn*.

* Space groups with different space-group numbers are non-isomorphic, except for the members of the 11 pairs of enantiomorphic space groups which are isomorphic.
† Subgroups belonging to the enantiomorphic space-group type of $\mathcal{G}$ are isomorphic to $\mathcal{G}$ and, therefore, are listed under **IIc** and not under **IIb**.

(ii) *Block* **IIb**

Whereas in blocks **I** and **IIa** *every* maximal subgroup $\mathcal{H}$ of $\mathcal{G}$ is listed, *this is no longer the case* for the entries of block **IIb**. The information given in this block is:

[*i*] HMS1 (Vectors) (HMS2, No.)

The symbols have the following meaning:

[*i*]: index of $\mathcal{H}$ in $\mathcal{G}$;

HMS1: Hermann–Mauguin symbol of $\mathcal{H}$, referred to the coordinate system and setting of $\mathcal{G}$; this symbol may be unconventional;*

(Vectors): basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of $\mathcal{H}$ in terms of the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of $\mathcal{G}$. No relations are given for unchanged axes, *e.g.* $\mathbf{a}' = \mathbf{a}$ is not stated;

(HMS2, No.): conventional short Hermann–Mauguin symbol, given only if HMS1 is not in conventional short form, and the space-group number of $\mathcal{H}$.

In addition to the general rule of increasing index [*i*] and decreasing space-group number (No.), the sequence of the **IIb** subgroups also depends on the type of cell enlargement. Subgroups with the same index and the same kind of cell enlargement are listed together in decreasing order of space-group number (see example 1 below).

In contradistinction to blocks **I** and **IIa**, for block **IIb** the coordinate triplets retained in $\mathcal{H}$ are *not* given. This means that the entry is the same for all subgroups $\mathcal{H}$ that have the same Hermann–Mauguin symbol and the same basis-vector relations to $\mathcal{G}$, but contain different sets of coordinate triplets. Thus, in block **IIb**, one entry may correspond to more than one subgroup,† as illustrated by the following examples.

Examples

(1) $\mathcal{G}$: $Pmm2$ (25)

IIb $\ldots$[2] $Pbm2$ ($\mathbf{b}' = 2\mathbf{b}$) ($Pma2$, 28); [2] $Pcc2$ ($\mathbf{c}' = 2\mathbf{c}$) (27);

$\ldots$[2] $Cmm2$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (35); $\ldots$

Each of the subgroups is referred to its own distinct basis $\mathbf{a}', \mathbf{b}'$, $\mathbf{c}'$, which is different in each case. Apart from the translations of the enlarged cell, the generators of the subgroups, referred to $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, are as follows:

$Pbm2$	x, y, z;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}+1/2, z$		or
	x, y, z;	$\bar{x}, \bar{y}+1/2, z$;	$x, \bar{y}, z$		
$Pcc2$	x, y, z;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}, z+1/2$		
$Cmm2$	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}, z$	or
	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}, z$;	$x, \bar{y}+1/2, z$	or
	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}+1/2, z$;	$x, \bar{y}, z$	or
	x, y, z;	$x+1/2, y+1/2, z$;	$\bar{x}, \bar{y}+1/2, z$;	$x, \bar{y}+1/2, z$.	

There are thus 2, 1 or 4 actual subgroups that obey the same basis-vector relations. The difference between the several subgroups represented by one entry is due to the different sets of symmetry operations of $\mathcal{G}$ that are retained in $\mathcal{H}$. This can also be expressed as different conventional origins of $\mathcal{H}$ with respect to $\mathcal{G}$.

(2) $\mathcal{G}$: $P3m1$ (156)

IIb $\ldots$[3] $H3m1$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($P31m$, 157)

The nine subgroups of type $P31m$ may be described in two ways:

(i) By partial 'decentring' of ninetuple cells ($\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$) with the same orientations as the cell of the group $\mathcal{G}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ in such a way that the centring points 0, 0, 0; $2/3, 1/3, 0$; $1/3, 2/3, 0$ (referred to $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$) are retained. The *conventional* space-group symbol $P31m$ of these nine subgroups is referred to the same basis vectors $\mathbf{a}'' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}'' = \mathbf{a} + 2\mathbf{b}$, $\mathbf{c}'' = \mathbf{c}$, but to different origins; *cf.* Section 2.2.15.5. This kind of description is used in the space-group tables of this volume.

(ii) Alternatively, one can describe the group $\mathcal{G}$ with an unconventional H-centred cell ($\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$) referred to which the space-group symbol is $H31m$. 'Decentring' of this cell results in the conventional space-group symbol $P31m$ for the subgroups, referred to the basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$. This description is used in Section 4.3.5.

(iii) *Subdivision of k subgroups into blocks* **IIa** *and* **IIb**

The subdivision of *k* subgroups into blocks **IIa** and **IIb** has no group-theoretical background and depends on the coordinate system chosen. The *conventional* coordinate system of the space group $\mathcal{G}$ (*cf.* Section 2.1.3) is taken as the basis for the subdivision. This results in a uniquely defined subdivision, except for the seven rhombohedral space groups for which in the space-group tables both 'rhombohedral axes' (primitive cell) and 'hexagonal axes' (triple cell) are given (*cf.* Section 2.2.2). Thus, some *k* subgroups of a rhombohedral space group are found under **IIa** (*klassengleich*, centring translations lost) in the *hexagonal* description, and under **IIb** (*klassengleich*, conventional cell enlarged) in the *rhombohedral* description.

Example: $\mathcal{G}$: $R\bar{3}$ (148) $\mathcal{H}$: $P\bar{3}$ (147)

Hexagonal axes

I	[2] $R3$ (146)	(1; 2; 3)+
	[3] $R\bar{1}$ ($P\bar{1}$, 2)	(1; 4)+
IIa {	[3] $P\bar{3}$ (147)	1; 2; 3; 4; 5; 6
	[3] $P\bar{3}$ (147)	1; 2; 3; (4; 5; 6) + $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$
	[3] $P\bar{3}$ (147)	1; 2; 3; (4; 5; 6) + $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$
IIb	none	

Rhombohedral axes

I	[2] $R3$ (146)	1; 2; 3
	[3] $R\bar{1}$ ($P\bar{1}$, 2)	1; 4
IIa	none	
IIb	[3] $P\bar{3}$ ($\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$) (147).	

Apart from the change from **IIa** to **IIb**, the above example demonstrates again the restricted character of the **IIb** listing, discussed above. The three conjugate subgroups $P\bar{3}$ of index [3] are listed under **IIb** by one entry only, because for all three subgroups the basis-vector relations between $\mathcal{G}$ and $\mathcal{H}$ are the same. Note the brace for the **IIa** subgroups, which unites *conjugate subgroups* into classes.

2.2.15.2. *Maximal isomorphic subgroups of lowest index (cf. Part 13)*

Another set of *klassengleiche* subgroups are the *isomorphic subgroups* listed under **IIc**, *i.e.* the subgroups $\mathcal{H}$ which are of the

* Unconventional Hermann–Mauguin symbols may include unconventional cells like *c* centring in quadratic plane groups, *F* centring in monoclinic, or *C* and *F* centring in tetragonal space groups. Furthermore, the triple hexagonal cells *h* and *H* are used for certain sub- and supergroups of the hexagonal plane groups and of the trigonal and hexagonal *P* space groups, respectively. The cells *h* and *H* are defined in Chapter 1.2. Examples are subgroups of plane groups $p3$ (13) and $p6mm$ (17) and of space groups $P3$ (143) and $P6/mcc$ (192).

† Without this restriction, the amount of data would be excessive. For instance, space group $Pmmm$ (47) has 63 maximal subgroups of index [2], of which seven are *t* subgroups and listed explicitly under **I**. The 16 entries under **IIb** refer to 50 actual subgroups and the one entry under **IIc** stands for the remaining 6 subgroups.

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 $\mathcal{G}$.* 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] $P3_212$ ($\mathbf{c}' = 2\mathbf{c}$) (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

$$P3_112 \rightarrow [2]\ P3_212\ (\mathbf{c}' = 2\mathbf{c}) \rightarrow [2]\ P3_112\ (\mathbf{c}'' = 2\mathbf{c}' = 4\mathbf{c}).$$

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

IIc [3] *Pnnm* ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (58); [3] *Pnnm* ($\mathbf{c}' = 3\mathbf{c}$) (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 $\mathcal{G}_1 = Pnnm$, 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 **b** and **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] *R*3 (obverse) (146); [3] *R*3 (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 **a**, **b**, **c**. In the *supergroup* data, $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are the basis vectors of the supergroup $\mathcal{S}$ and **a**, **b**, **c** are again the basis vectors of $\mathcal{G}$. Thus, **a**, **b**, **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, $\mathbf{c}(Pna2_1) = 2\mathbf{c}(Pba2)$.

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

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)

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

Thus, the basis vectors of the supergroup are

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

An alternative description is

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

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

(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

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

An alternative description is

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

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

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 **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.

* 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.

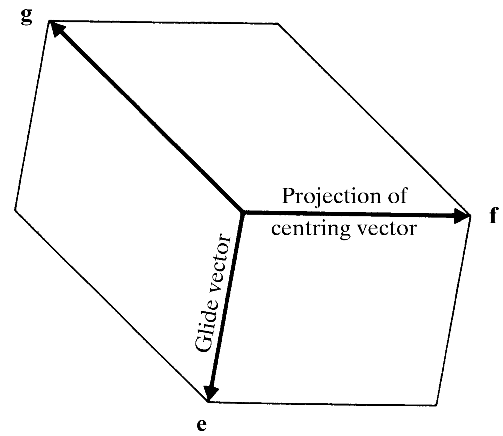

Fig. 2.2.16.1. The three primitive two-dimensional cells which are spanned by the shortest three translation vectors **e**, **f**, **g** in the monoclinic plane. For the present discussion, the glide vector is considered to be along **e** and the projection of the centring vector along **f**.

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.

† 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.

references