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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 *c*2*mm* (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 *p*2*gm* (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) $\mathcal{G}$: *C*1*m*1 (8)

I	[2] *C*1 (*P*1, 1)	1+
IIa	[2] *P*1*a*1 (*Pc*, 7)	1; 2 + (1/2, 1/2, 0)
	[2] *P*1*m*1 (*Pm*, 6)	1; 2

where the numbers have the following meaning:

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

(2) $\mathcal{G}$: *Fdd*2 (43)

I [2] *F*112 (*C*2, 5) (1; 2)+

where the numbers have the following meaning:

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

(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.

references