1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

Table 1.2.14.2. *Projection of three-dimensional symmetry elements (layer and rod groups)*

Symmetry element in three dimensions		Symmetry element in projection	
Arbitrary orientation			
Symmetry centre $\bar{1}$		Rotation point 2 at projection of centre	
Parallel to projection direction			
Rotation axis	2, 3, 4, 6	Rotation point	2, 3, 4, 6
Screw axis	2_1	Rotation point	2
	$3_1, 3_2$		3
	$4_1, 4_2, 4_3$		4
	$6_1, 6_2, 6_3, 6_4, 6_5$		6
Rotoinversion axis	$\bar{4}$	Rotation point	4
	$\bar{6} \equiv 3/m$		3 (with overlap of atoms)
	$\bar{3} \equiv 3 \times \bar{1}$		6
Reflection plane *m*		Reflection line *m*	
Glide plane with $\perp$ component†		Glide line *g*	
Glide plane without $\perp$ component†		Reflection line *m*	
Normal to projection direction			
Rotation axis	2, 4, 6	Reflection line *m*	
	3	None	
Screw axis	$4_2, 6_2, 6_4$	Reflection line *m*	
	$2_1, 4_1, 4_3, 6_1, 6_3, 6_5$	Glide line *g*	
	$3_1, 3_2$	None	
Rotoinversion axis	$\bar{4}$	Reflection line *m* parallel to axis	
	$\bar{6} \equiv 3/m$	Reflection line *m* perpendicular to axis	
	$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)	
Reflection plane *m*		None, but overlap of atoms	
Glide plane with glide component **t**		Translation **t**	

† The term 'with $\perp$ component' refers to the component of the glide vector normal to the projection direction.

(iv) *Location of the origin* of the plane group, frieze group and one-dimensional space group is given with respect to the conventional lattice of the subperiodic group. The same description is used as for the location of symmetry elements (see Section 1.2.9). *Example*: 'Origin at *x*, 0, 0' or 'Origin at *x*, 1/4, 0'.

1.2.14.2. Projections of centred subperiodic groups

The only centred subperiodic groups are the nine types of centred layer groups. For the [100] and [010] projection directions, because of the centred layer-group lattice, the basis vectors of the resulting frieze groups are $\mathbf{a}' = \mathbf{b}/2$ and $\mathbf{a}' = \mathbf{a}/2$, respectively.

1.2.14.3. Projection of symmetry elements

A symmetry element of a subperiodic group projects as a symmetry element only if its orientation bears a special relationship to the projection direction. In Table 1.2.14.2, the three-dimensional symmetry elements of the layer and rod groups and in Table 1.2.14.3 the two-dimensional symmetry elements of the frieze groups are listed along with the corresponding symmetry element in projection.

Example: Layer group cm2m (L35)

Projection along [001]: This orthorhombic/rectangular plane group is centred; *m* perpendicular to [100] is projected as a reflection line, 2 parallel to [010] is projected as the same reflection line and *m* perpendicular to [001] gives rise to no symmetry element in projection, but to an overlap of atoms. *Result*: Plane group *c*1*m*1 (5) with $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$.

Projection along [100]: The frieze group has the basis vector $\mathbf{a}'$ = $\mathbf{b}/2$ due to the centred lattice of the layer group. *m* perpendicular to [100] gives rise only to an overlap of atoms, 2 parallel to [010] is projected as a reflection line and *m* perpendicular to [001] is projected as the same reflection line. *Result*: Frieze group *⁀*11*m* (F4) with $\mathbf{a}' = \mathbf{b}/2$.

Projection along [010]: The frieze group has the basis vector $\mathbf{a}'$ = $\mathbf{a}/2$ due to the centred lattice of the layer group. The two reflection planes project as perpendicular reflection lines and 2 parallel to [010] projects as the rotation point 2. *Result*: Frieze group *⁀*2*mm* (F6) with $\mathbf{a}' = \mathbf{a}/2$.

1.2.15. Maximal subgroups and minimal supergroups

In *IT* A (2005), for the representative space group of each space-group type the following information is given:

(i) maximal non-isomorphic subgroups,

(ii) maximal isomorphic subgroups of lowest index,

(iii) minimal non-isomorphic supergroups and

(iv) minimal isomorphic supergroups of lowest index.

However, Bieberbach's theorem for space groups, *i.e.* the classification into isomorphism classes is identical with the classification into affine equivalence classes, is not valid for subperiodic groups. Consequently, to obtain analogous tables for the subperiodic groups, we provide the following information for each representative subperiodic group:

(i) maximal non-isotypic non-enantiomorphic subgroups,

(ii) maximal isotypic subgroups and enantiomorphic subgroups of lowest index,

1. SUBPERIODIC GROUP TABLES: FRIEZE-GROUP, ROD-GROUP AND LAYER-GROUP TYPES

Table 1.2.14.3. *Projection of two-dimensional symmetry elements (frieze groups)*

Symmetry element in two dimensions	Symmetry element in projection
Rotation point 2	Reflection point m
Parallel to projection direction	
Reflection line m	Reflection point m
Glide line g	Reflection point m
Normal to projection direction	
Reflection line m	None (with overlap of atoms)
Glide line g with glide component $\mathbf{t}$	Translation $\mathbf{t}$

(iii) minimal non-isotypic non-enantiomorphic supergroups and

(iv) minimal isotypic supergroups and enantiomorphic supergroups of lowest index,

where *isotypic* means 'belonging to the same subperiodic group type'. The cases of maximal enantiomorphic subgroups of lowest index and minimal enantiomorphic supergroups of lowest index arise only in the case of rod groups.

1.2.15.1. Maximal non-isotypic non-enantiomorphic subgroups

The maximal non-isotypic non-enantiomorphic subgroups **S** of a subperiodic group **G** are divided into two types:

I *translationengleiche* or *t* subgroups and

II *klassengleiche* or *k* subgroups.

Type **II** is subdivided again into two blocks:

IIa: the conventional cells of **G** and **S** are the same, and

IIb: the conventional cell of **S** is larger than that of **G**.

Block **IIa** has no entries for subperiodic groups with a primitive cell. Only in the case of the nine centred layer groups are there entries, when it contains those maximal subgroups **S** which have lost all the centring translations of **G** but none of the integral translations.

1.2.15.1.1. Blocks **I** and **IIa**

In blocks **I** and **IIa**, *every* maximal subgroup **S** of a subperiodic group **G** is listed with the following information:

[*i*]   HMS1   (HMS2)   Sequence of numbers

The symbols have the following meaning:

[*i*]: index of **S** in **G**.

HMS1: short Hermann–Mauguin symbol of **S**, referred to the coordinate system and setting of **G**; this symbol may be unconventional.

(HMS2): conventional short Hermann–Mauguin symbol of **S**, given only if HMS1 is not in conventional short form.

Sequence of numbers: coordinate triplets of **G** retained in **S**. The numbers refer to the numbering scheme of the coordinate triplets of the general position. For the centred layer groups the following abbreviations are used:

Block **I** (all translations retained). *Number* +: coordinate triplet given by *Number*, plus that obtained by adding the centring translation (1/2, 1/2, 0) of **G**. (*Numbers*) +: the same as above, but applied to all *Numbers* between parentheses.

Block **IIa** (not all translations retained). *Number* + (1/2, 1/2, 0): coordinate triplet obtained by adding the translation (1/2, 1/2, 0):

to the triplet given by *Number*. (*Numbers*) + (1/2, 1/2, 0): the same as above, but applied to all *Numbers* between parentheses.

Examples

(1) **G**: Layer group $c211$ (L10)

I	[2]	$c1\,(p1)$	$1+$
IIa	[2]	$p2_111$	$1; 2 + (1/2, 1/2, 0)$
	[2]	$p211$	$1; 2$

where the numbers have the following meaning:

$$
\begin{array}{lll}
1+ & x, y, z & x + 1/2, y + 1/2, z \\
1; 2 & x, y, z & x, \bar{y}, \bar{z} \\
1; 2+ & x, y, z & x + 1/2, \bar{y} + 1/2, \bar{z}
\end{array}
$$

(2) **G**: Rod group $\textit{p}422$ (R30)

I	[2]	$\textit{p}411\,(\textit{p}4)$	$1; 2; 3; 4$
	[2]	$\textit{p}221\,(\textit{p}222)$	$1; 2; 5; 6$
	[2]	$\textit{p}212\,(\textit{p}222)$	$1; 2; 7; 8$

The HMS1 symbol in each of the three subgroups **S** is given in the tetragonal coordinate system of the group **G**. In the first case, $\textit{p}411$ is not the conventional short Hermann–Mauguin symbol and a second conventional symbol $\textit{p}4$ is given. In the latter two cases, since the subgroups are orthorhombic rod groups, a second conventional symbol of the subgroup in an orthorhombic coordinate system is given.

1.2.15.1.2. Block **IIb**

Whereas in blocks **I** and **IIa** *every* maximal subgroup **S** of **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)

The symbols have the following meaning:

[*i*]: index of **S** in **G**.

HMS1: Hermann–Mauguin symbol of **S**, referred to the coordinate system and setting of **G**; this symbol may be unconventional.

(Vectors): basis vectors of **S** in terms of the basis vectors of **G**. No relations are given for basis vectors which are unchanged.

(HMS2): conventional short Hermann–Mauguin symbol, given only if HMS1 is not in conventional short form.

Examples

(1) **G**: Rod group $\textit{p}222$ (R13)

IIb	$[2]\,\textit{p}222_1\;(\mathbf{c}' = 2\mathbf{c})$

There are two subgroups which obey the same basis-vector relation. Apart from the translations of the enlarged cell, the generators of the subgroups, referred to the basis vectors of the enlarged cell, are

$$
\begin{array}{llll}
x, y, z & x, \bar{y}, \bar{z} + 1/2 & \bar{x}, y, \bar{z} \\
x, y, z & x, \bar{y}, \bar{z} & \bar{x}, y, \bar{z} + 1/2.
\end{array}
$$

(2) **G**: Layer group $pm2_1b$ (L28)

IIb	$[2]\,pm2_1n\;(\mathbf{a}' = 2\mathbf{a})$

This entry represents two subgroups whose generators, apart from the translations of the enlarged cell, are

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

The difference between the two subgroups represented by the one entry is due to the different sets of symmetry operations of **G** which are retained in **S**. This can also be expressed as different conventional origins of **S** with respect to **G**: the two subgroups in the first example above are related by a translation **c**/4 of the origin, and the two subgroups in the second example by **a**/4.

1.2.15.2. Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

Another set of *klassengleiche* subgroups is that listed under **IIc**, *i.e.* the subgroups **S** which are of the same or of the enantiomorphic subperiodic group type as **G**. Again, one entry may correspond to more than one isotypic subgroup:

(*a*) As in block **IIb**, one entry may correspond to two isotypic subgroups whose difference can be expressed as different conventional origins of **S** with respect to **G**.

(*b*) One entry may correspond to two isotypic subgroups of equal index but with cell enlargements in different directions which are conjugate subgroups in the affine normalizer of **G**. The different vector relationships are given, separated by 'or' and placed within one pair of parentheses; *cf.* example (2).

Examples

(1) **G**: Rod group $p222$ (R13)
   IIc [2] $p222$ ($\mathbf{c}' = 2\mathbf{c}$)

This entry corresponds to two isotypic subgroups. Apart from the translations of the enlarged cell, the generators of the subgroups are

$$x, y, z \quad x, \bar{y}, \bar{z} \quad \bar{x}, y, \bar{z}$$
$$x, y, z \quad x, \bar{y}, \bar{z} + 1/2 \quad \bar{x}, y, \bar{z} + 1/2$$

(2) **G**: Layer group $pmm2$ (L23)
   IIc [2] $pmm2$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$)

This entry corresponds to four isotypic subgroups, two with the enlarged cell with $\mathbf{a}' = 2\mathbf{a}$ and two with the enlarged cell with $\mathbf{b}' = 2\mathbf{b}$. The generators of these subgroups are

$\mathbf{a}' = 2\mathbf{a}$	$\mathbf{b}' = \mathbf{b}$	x, y, z	$\bar{x}, y, z$	$x, \bar{y}, z$
$\mathbf{a}' = 2\mathbf{a}$	$\mathbf{b}' = \mathbf{b}$	x, y, z	$\bar{x} + 1/2, y, z$	$x, \bar{y}, z$
$\mathbf{a}' = \mathbf{a}$	$\mathbf{b}' = 2\mathbf{b}$	x, y, z	$\bar{x}, y, z$	$x, \bar{y}, z$
$\mathbf{a}' = \mathbf{a}$	$\mathbf{b}' = 2\mathbf{b}$	x, y, z	$\bar{x}, y + 1/2, z$	$x, \bar{y}, z$

(3) **G**: Rod group $p4_1$ (R24)
   IIc [3] $p4_3$ ($\mathbf{c}' = 3\mathbf{c}$)
         [5] $p4_1$ ($\mathbf{c}' = 5\mathbf{c}$)

Listed here are both the maximal isotypic subgroup $p4_1$ and the maximal enantiomorphic subgroup $p4_3$, each of lowest index.

1.2.15.3. Minimal non-isotypic non-enantiomorphic supergroups

If **G** is a maximal subgroup of a group **H**, then **H** is called a minimal supergroup of **G**. Minimal supergroups are again subdivided into two types, the *translationengleiche* or *t* supergroups **I** and the *klassengleiche* or *k* supergroups **II**. For the *t* supergroups **I** of **G**, the listing contains the index [*i*] of **G** in **H** and

the *conventional* Hermann–Mauguin symbol of **H**. For the *k* supergroups **II**, the subdivision between **IIa** and **IIb** is not made. The information given is similar to that for the subgroups **IIb**, *i.e.* the relations between the basis vectors of group and supergroup are given, in addition to the Hermann–Mauguin symbols of **H**. Note that either the conventional cell of the *k* supergroup **H** is smaller than that of the subperiodic group **G**, or **H** contains additional centring translations.

*Example: **G**: Layer group $p2_1/m11$ (L15)*
   Minimal non-isotypic non-enantiomorphic supergroups:

   I   [2]$pmam$; [2]$pmma$; [2]$pbma$; [2]$pmmn$

   II [2]$c2/m11$; [2]$p2/m11$ ($2\mathbf{a}' = \mathbf{a}$)

Block **I** lists [2] *pmam*, [2] *pmma* and [2] *pmmn*. Looking up the *subgroup* data of these three groups one finds [2] $p2_1/m11$. Block **I** also lists [2] *pbma*. Looking up the *subgroup* data of this group one finds [2] $p12_1/m1$ ($p2_1/m11$). This shows that the setting of *pbma* does not correspond to that of $p2_1/m11$ but rather to $p12_1/m1$. To obtain the supergroup **H** referred to the basis of $p2_1/m11$, the basis vectors **a** and **b** must be interchanged. This changes *pbma* to *pmba*, which is the correct symbol of the supergroup of $p2_1/m11$.

Block **II** contains two entries: the first where the conventional cells are the same with the supergroup having additional centring translations, and the second where the conventional cell of the supergroup is smaller than that of the original subperiodic group.

1.2.15.4. Minimal isotypic supergroups and enantiomorphic supergroups of lowest index

No data are listed for *supergroups* **IIc**, because they can be derived directly from the corresponding data of *subgroups* **IIc**.

*Example: **G**: Rod group $p4_2/m$ (R29)*
   The maximal isotypic subgroup of lowest index of $p4_2/m$ is found in block **IIc**: [3] $p4_2/m$ ($\mathbf{c}' = 3\mathbf{c}$). By interchanging $\mathbf{c}'$ and **c**, one obtains the minimal isotypic supergroup of lowest index, *i.e.* [3] $p4_2/m$ ($3\mathbf{c}' = \mathbf{c}$).

1.2.16. Nomenclature

There exists a wide variety of nomenclature for layer, rod and frieze groups (Holser, 1961). Layer-group nomenclature includes *zweidimensionale Raumgruppen* (Alexander & Herrmann, 1929*a*,*b*), *Ebenengruppen* (Weber, 1929), *Netzgruppen* (Hermann, 1929*a*), *net groups* (*IT*, 1952; Opechowski, 1986), *reversal space groups in two dimensions* (Cochran, 1952), *plane groups in three dimensions* (Dornberger-Schiff, 1956, 1959; Belov, 1959), *black and white space groups in two dimensions* (Mackay, 1957), (*two-sided*) *plane groups* (Holser, 1958), *Schichtgruppen* (Niggli, 1959; Chapuis, 1966), *diperiodic groups in three dimensions* (Wood, 1964*a*,*b*), *layer space groups* (Shubnikov & Koptsik, 1974), *layer groups* (Köhler, 1977; Koch & Fischer, 1978; Vainshtein, 1981; Goodman, 1984; Litvin, 1989), *two-dimensional (subperiodic) groups in three-dimensional space* (Brown *et al.*, 1978) and *plane space groups in three dimensions* (Grell *et al.*, 1989).

Rod-group nomenclature includes *Kettengruppen* (Hermann, 1929*a*,*b*), *eindimensionalen Raumgruppen* (Alexander, 1929, 1934), (*crystallographic*) *line groups in three dimensions* (*IT*, 1952; Opechowski, 1986), *rod groups* (Belov, 1956; Vujicic *et al.*, 1977; Köhler, 1977; Koch & Fischer, 1978), *Balkengruppen*

references