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additional centring translation $t(1/2, 1/2, 0)$. The additional generators are given as numbers (p) which refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*; for centred layer groups, the first block 'For (0, 0, 0)+ set' must be used.

1.2.11. Positions

The entries under *Positions* (more explicitly called *Wyckoff positions*) consist of the *General position* (upper block) and the *Special positions* (blocks below). The columns in each block, from left to right, contain the following information for each Wyckoff position.

(i) *Multiplicity M* of the Wyckoff position. This is the number of equivalent points per conventional cell. The multiplicity M of the general position is equal to the order of the point group of the subperiodic group, except in the case of centred layer groups when it is twice the order of the point group. The multiplicity M of a special position is equal to the order of the point group of the subperiodic group divided by the order of the site-symmetry group (see Section 1.2.12).

(ii) *Wyckoff letter*. This letter is a coding scheme for the Wyckoff positions, starting with a at the bottom position and continuing upwards in alphabetical order.

(iii) *Site symmetry*. This is explained in Section 1.2.12.

(iv) *Coordinates*. The sequence of the coordinate triplets is based on the *Generators*. For the centred layer groups, the centring translations (0, 0, 0)+ and (1/2, 1/2, 0)+ are listed above the coordinate triplets. The symbol '+' indicates that in order to obtain a complete Wyckoff position, the components of these centring translations have to be added to the listed coordinate triplets.

(v) *Reflection conditions*. These are described in Section 1.2.13.

The two types of positions, general and special, are characterized as follows:

(i) *General position*. A set of symmetrically equivalent points is said to be in a 'general position' if each of its points is left invariant only by the identity operation but by no other symmetry operation of the subperiodic group.

(ii) *Special position(s)*. A set of symmetrically equivalent points is said to be in a 'special position' if each of its points is mapped onto itself by at least one additional operation in addition to the identity operation.

Example: Layer group $c2/m11$ (L18)

The general position $8f$ of this layer group contains eight equivalent points per cell each with site symmetry 1. The coordinate triplets of four points (1) to (4) are given explicitly, the coordinate triplets of the other four points are obtained by adding the components (1/2, 1/2, 0) of the c-centring translation to the coordinate triplets (1) to (4).

This layer group has five special positions with the Wyckoff letters a to e. The product of the multiplicity and the order of the site-symmetry group is the multiplicity of the general position. For position $4d$, for example, the four equivalent points have the coordinates $x, 0, 0,\ \bar{x}, 0, 0,\ x+1/2, 1/2, 0$ and $\bar{x}+1/2, 1/2, 0$. Since each point of position $4d$ is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from eight to four, whereas the order of the site symmetry is increased from one to two.

1.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *site symmetry* of that position. The site-symmetry group is isomorphic to a proper or improper subgroup of the point group to which the subperiodic group under consideration belongs. *Oriented site-symmetry symbols* are used to show how the symmetry elements at a site are related to the conventional crystallographic basis. The site-symmetry symbols display the same sequence of symmetry directions as the subperiodic group symbol (*cf.* Table 1.2.4.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the $2c$ position of tetragonal layer group $p4mm$ (L55), the site-symmetry group is the orthorhombic group '$2mm.$'. The two characters 'mm' represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry direction.

1.2.13. Reflection conditions

The *Reflection conditions* are listed in the right-hand column of each Wyckoff position. There are two types of reflection conditions:

(i) *General conditions*. These conditions apply to *all* Wyckoff positions of the subperiodic group.

(ii) *Special conditions* ('extra' conditions). These conditions apply only to *special* Wyckoff positions and must always be added to the general conditions of the subperiodic group.

The *general reflection conditions* are the result of three effects: centred lattices, glide planes and screw axes. For the nine layer groups with *centred* lattices, the corresponding general reflection condition is $h+k=2n$. The general reflection conditions due to glide planes and screw axes for the subperiodic groups are given in Table 1.2.13.1.

Example: The layer group $p4bm$ (L56)

General position $8d$: $0k: k=2n$ and $h0: h=2n$ due respectively to the glide planes b and a. The projections along [100] and [010] of any crystal structure with this layer-group symmetry have, respectively, periodicity $\mathbf{b}/2$ and $\mathbf{a}/2$.

Special positions $2a$ and $2b$: $hk: h+k=2n$. Any set of equivalent atoms in either of these positions displays additional c-centring.

1.2.14. Symmetry of special projections

1.2.14.1. *Data listed in the subperiodic group tables*

Under the heading *Symmetry of special projections*, the following data are listed for three orthogonal projections of each layer group and rod group and two orthogonal projections of each frieze group:

(i) For layer and rod groups, each projection is made onto a plane normal to the projection direction. If there are three kinds of symmetry directions (*cf.* Table 1.2.4.1), the three projection directions correspond to the primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction(s) are taken along coordinate axes.

For frieze groups, each projection is made on a line normal to the projection direction.

The directions for which data are listed are as follows:

(*a*) *Layer groups*:

Triclinic/oblique	[001][100][010]
Monoclinic/oblique	[001][100][010]
Monoclinic/rectangular	[001][100][010]
Orthorhombic/rectangular	[001][100][010]
Tetragonal/square	[001][100][110]
Trigonal/hexagonal	[001][100][210]
Hexagonal/hexagonal	[001][100][210]

(*b*) *Rod groups*:

Triclinic Monoclinic/inclined Monoclinic/orthogonal Orthorhombic	[001][100][010]
Tetragonal	[001][100][110]
Trigonal Hexagonal	[001][100][210]

(*c*) *Frieze groups*:

Oblique Rectangular	[10][01]

(ii) *The Hermann–Mauguin symbol*. For the [001] projection of a layer group, the Hermann–Mauguin symbol for the plane group resulting from the projection of the layer group is given. For the [001] projection of a rod group, the Hermann–Mauguin symbol for the resulting two-dimensional point group is given. For the remainder of the projections, in the case of both layer groups and rod groups, the Hermann–Mauguin symbol is given for the resulting frieze group. For the [10] projection of a frieze group, the Hermann–Mauguin symbol of the resulting one-dimensional point group, *i.e.* 1 or *m*, is given. For the [01] projection, the Hermann–Mauguin symbol of the resulting one-dimensional space group, *i.e.* *p*1 or *pm*, is given.

(iii) For layer groups, the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ of the plane group resulting from the [001] projection and the basis vector $\mathbf{a}'$ of the frieze groups resulting from the additional two projections are given as linear combinations of the basis vectors **a**, **b** of the layer group. Basis vectors **a**, **b** inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p$, $\mathbf{b}_p$. For the two projections of a rod group resulting in a frieze group, the basis vector $\mathbf{a}'$ of the resulting frieze group is given in terms of the basis vector **c** of the rod group. For the [01] projection of a frieze group, the basis vector $\mathbf{a}'$ of the resulting one-dimensional space group is given in terms of the basis vector **a** of the frieze group.

For rod groups and layer groups, the relations between a', b' and γ' of the projected conventional basis vectors and a, b, c, α, β and γ of the conventional basis vectors of the subperiodic group are given in Table 1.2.14.1. We also give in this table the relations between a' of the projected conventional basis and a, b and γ of the conventional basis of the frieze group.

(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.

Table 1.2.13.1. *General reflection conditions due to glide planes and screw axes*

(*a*) Layer groups.

(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
hk: $h = 2n$	(001)	$\mathbf{a}/2$	a
hk: $k = 2n$	(001)	$\mathbf{b}/2$	b
hk: $h + k = 2n$	(001)	$\mathbf{a}/2 + \mathbf{b}/2$	n
$0k$: $k = 2n$	(100)	$\mathbf{b}/2$	b
$h0$: $h = 2n$	(010)	$\mathbf{a}/2$	a

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
$h0$: $h = 2n$	[100]	$\mathbf{a}/2$	2_1
$0k$: $k = 2n$	[010]	$\mathbf{b}/2$	2_1

(*b*) Rod groups.

(1) Glide planes.

Reflection condition	Orientation of plane	Glide vector	Symbol
l: $l = 2n$	Any orientation parallel to the c axis	$\mathbf{c}/2$	c

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
l: $l = 2n$	[001]	$\mathbf{c}/2$	2_1, 4_2, 6_3
l: $l = 3n$	[001]	$\mathbf{c}/3$	3_1, 3_2, 6_2, 6_4
l: $l = 4n$	[001]	$\mathbf{c}/4$	4_1, 4_3
l: $l = 6n$	[001]	$\mathbf{c}/6$	6_1, 6_5

(*c*) Frieze groups, glide plane.

Reflection condition	Orientation of plane	Glide vector	Symbol
h: $h = 2n$	(10)	$\mathbf{a}/2$	g

Example: Layer group *cm*2*m* (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 $\not{p}11m$ (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 $\not{p}2mm$ (F6) with $\mathbf{a}' = \mathbf{a}/2$.

1.2.15. Maximal subgroups and minimal supergroups

In *IT* A (1983), for the representative space group of each space-group type the following information is given:

(i) maximal non-isomorphic subgroups,

references