International Tables for Crystallography (2010). Vol. E, Section 1.2.12, pp. 16–17.

translations to each printed coordinate triplet in order to obtain the complete general position. For the *Symmetry operations*, the corresponding data are listed explicitly with the two blocks having the subheadings 'For (0, 0, 0)+ set' and 'For (1/2, 1/2, 0)+ set', respectively.

1.2.9.2. Designation of symmetry operations

The designation of symmetry operations for the subperiodic groups is the same as for the space groups. An entry in the block *Symmetry operations* is characterized as follows:

(i) A symbol denoting the *type* of the symmetry operation [*cf*. Chapter 1.2 of *IT* A (2005)], including its glide or screw part, if present. In most cases, the glide or screw part is given explicitly by fractional coordinates between parentheses. The sense of a rotation is indicated by the superscript + or −. Abbreviated notations are used for the glide reflections $a(1/2, 0, 0) \equiv a$; $b(0, 1/2, 0) \equiv b$; $c(0, 0, 1/2) \equiv c$. Glide reflections with complicated and unconventional glide parts are designated by the letter g, followed by the glide part between parentheses.

(ii) A coordinate triplet indicating the *location* and *orientation* of the symmetry element which corresponds to the symmetry operation. For rotoinversions the location of the inversion point is also given.

Details of this symbolism are given in Section 11.1.2 of *IT* A (2005).

Examples

(1) $m \quad x, 0, z$: a reflection through the plane $x, 0, z$, *i.e.* the plane parallel to (010) containing the point (0, 0, 0).

(2) $m \quad x + 1/2, \bar{x}, z$: a reflection through the plane $x + 1/2, \bar{x}, z$, *i.e.* the plane parallel to (110) containing the point (1/2, 0, 0).

(3) $g(1/2, 1/2, 0) \quad x, x, z$: glide reflection with glide component (1/2, 1/2, 0) through the plane x, x, z, *i.e.* the plane parallel to $(1\bar{1}0)$ containing the point (0, 0, 0).

(4) $2(1/2, 0, 0) \quad x, 1/4, 0$: screw rotation along the (100) direction containing the point (0, 1/4, 0) with a screw component (1/2, 0, 0).

(5) $\bar{4}^{-} \quad 1/2, 0, z \quad 1/2, 0, 0$: fourfold rotoinversion consisting of a clockwise rotation by 90° around the line $1/2, 0, z$ followed by an inversion through the point (1/2, 0, 0).

1.2.10. Generators

The line *Generators selected* states the symmetry operations and their sequence selected to generate all symmetrically equivalent points of the *General position* from a point with coordinates x, y, z. The identity operation given by (1) is always selected as the first generator. The generating translations are listed next, $t(1, 0)$ for frieze groups, $t(0, 0, 1)$ for rod groups, and $t(1, 0, 0)$ and $t(0, 1, 0)$ for layer groups. For centred layer groups, there is the 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

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)	**a**/2	*a*
hk: $k = 2n$	(001)	**b**/2	*b*
hk: $h + k = 2n$	(001)	**a**/2 + **b**/2	*n*
$0k$: $k = 2n$	(100)	**b**/2	*b*
$h0$: $h = 2n$	(010)	**a**/2	*a*

(2) Screw axes.

Reflection condition	Direction of axis	Screw vector	Symbol
$h0$: $h = 2n$	[100]	**a**/2	2_1
$0k$: $k = 2n$	[010]	**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	**c**/2	*c*

(2) Screw axes.

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

(*c*) Frieze groups, glide plane.

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

the site-symmetry group belongs to a lower crystal system. For example, for the 2*c* position of tetragonal layer group *p*4*mm* (L55), the site-symmetry group is the orthorhombic group '2*mm*.'. 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 8*d*: $0k: k = 2n$ 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 **b**/2 and **a**/2.

Special positions 2*a* and 2*b*: $hk: h + k = 2n$. 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 Monoclinic/oblique Monoclinic/rectangular Orthorhombic/rectangular	[001], [100], [010]
Tetragonal/square	[001], [100], [110]
Trigonal/hexagonal 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

references