1.2. Guide to the use of the subperiodic group tables

This present volume is, in part, an extension of *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (*IT* A, 1983). Symmetry tables are given in *IT* A for the 230 three-dimensional crystallographic space-group types (space groups) and the 17 two-dimensional crystallographic space-group types (plane groups). We give in the following three parts of this volume analogous symmetry tables for the two-dimensional and three-dimensional subperiodic group types: the seven crystallographic *frieze-group* types (two-dimensional groups with one-dimensional translations) in Part 2; the 75 crystallographic *rod-group* types (three-dimensional groups with one-dimensional translations) in Part 3; and the 80 crystallographic *layer-group* types (three-dimensional groups with two-dimensional translations) in Part 4. This chapter forms a guide to the entries of the subperiodic group tables given in Parts 2–4.

1.2.1. Classification of subperiodic groups

Subperiodic groups can be classified in ways analogous to the space groups. For the mathematical definitions of these classifications and their use for space groups, see Section 8.2 of *IT* A (1983). Here we shall limit ourselves to those classifications which are explicitly used in the symmetry tables of the subperiodic groups.

1.2.1.1. *Subperiodic group types*

The subperiodic groups are classified into *affine subperiodic group types*, *i.e.* affine equivalence classes of subperiodic groups. There are 80 affine layer-group types and seven affine frieze-group types. There are 67 crystallographic and an infinity of noncrystallographic affine rod-group types. We shall consider here only rod groups of the 67 crystallographic rod-group types and refer to these crystallographic affine rod-group types simply as affine rod-group types.

The subperiodic groups are also classified into *proper affine subperiodic group types*, *i.e.* proper affine classes of subperiodic groups. For layer and frieze groups, the two classifications are identical. For rod groups, each of eight affine rod-group types splits into a pair of *enantiomorphic crystallographic rod-group types*. Consequently, there are 75 proper affine rod-group types. The eight pairs of enantiomorphic rod-group types are $\not{p}4_1$ (R24), $\not{p}4_3$ (R26); $\not{p}4_122$ (R31), $\not{p}4_322$ (R33); $\not{p}3_1$ (R43), $\not{p}3_2$ (R44); $\not{p}3_112$ (R47), $\not{p}3_212$ (R48); $\not{p}6_1$ (R54), $\not{p}6_5$ (R58); $\not{p}6_2$ (R55), $\not{p}6_4$ (R57); $\not{p}6_122$ (R63), $\not{p}6_522$ (R67); and $\not{p}6_222$ (R64), $\not{p}6_422$ (R66). (Each subperiodic group is given in the text by its Hermann–Mauguin symbol followed in parenthesis by a letter L, R or F to denote it, respectively, as a layer, rod or frieze group, and its sequential numbering from Parts 2, 3 or 4.) We shall refer to the proper affine subperiodic group types simply as subperiodic group types.

1.2.1.2. *Other classifications*

There are 27 geometric crystal classes of layer groups and rod groups, and four geometric crystal classes of frieze groups. These are listed, for layer groups, in the fourth column of Table 1.2.1.1, and for the rod and frieze groups in the second columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

We further classify subperiodic groups according to the following classifications of the subperiodic group's point group and lattice group. These classifications are introduced to emphasize the relationships between subperiodic groups and space groups:

(1) The point group of a layer or rod group is three-dimensional and corresponds to a point group of a three-dimensional space group. The point groups of three-dimensional space groups are classified into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic crystal systems. We shall use this classification also for subperiodic groups. Consequently, the three-dimensional subperiodic groups are classified, see the third column of Table 1.2.1.1 and the first column of Table 1.2.1.2, into the triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal crystal systems. The cubic crystal system does not arise for three-dimensional subperiodic groups. Two-dimensional subperiodic groups, *i.e.* frieze groups, are analogously classified, see the first column of Table 1.2.1.3, into the oblique and rectangular crystal systems.

(2) The two-dimensional lattice of a layer group is also a two-dimensional lattice of a plane group. The lattices of plane groups are classified, according to *Bravais* (*flock*) *systems*, see *IT* A (1983), into the oblique, rectangular, square and hexagonal Bravais systems. We shall also use this classification for layer groups, see the first column in Table 1.2.1.1. For rod and frieze groups no lattice classification is used, as all one-dimensional lattices form a single Bravais system.

A subdivision of the monoclinic rod-group category is made into monoclinic/inclined and monoclinic/orthogonal. Two different coordinate systems, see Table 1.2.1.2, are used for the rod groups of these two subdivisions of the monoclinic crystal system. These two coordinate systems differ in the orientation of the plane containing the non-lattice basis vectors relative to the lattice vectors. For the monoclinic/inclined subdivision, the plane containing the non-lattice basis vectors is, see Fig. 1.2.1.1, *inclined* with respect to the lattice basis vector. For the monoclinic/orthogonal subdivision, the plane is, see Fig. 1.2.1.2, *orthogonal*.

1.2.1.2.1. *Conventional coordinate systems*

The subperiodic groups are described by means of a *crystallographic coordinate system* consisting of a *crystallographic origin*, denoted by O, and a *crystallographic basis*. The basis vectors for the three-dimensional layer groups and rod groups are labelled **a**, **b** and **c**. The basis vectors for the two-dimensional frieze groups are labelled **a** and **b**. Unlike space groups, not all basis vectors of the crystallographic basis are lattice vectors. Like space groups, the crystallographic coordinate system is used to define the symmetry operations (see Section 1.2.9) and the Wyckoff positions (see Section 1.2.11). The symmetry operations are defined with respect to the directions of both lattice and non-lattice basis vectors. A Wyckoff position, denoted by a coordinate triplet (x, y, z) for the three-dimensional layer and rod groups, is defined in the crystallographic coordinate system by $O + \mathbf{r}$, where $\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$. For the two-dimensional frieze groups, a Wyckoff position is denoted by a coordinate doublet (x, y) and is defined in the crystallographic coordinate system by $O + \mathbf{r}$, where $\mathbf{r} = x\mathbf{a} + y\mathbf{b}$.

The term *setting* will refer to the assignment of the labels **a**, **b** and **c** (and the corresponding directions [100], [010] and [001], respectively) to the basis vectors of the crystallographic basis (see Section 1.2.6). In the *standard setting*, those basis vectors which are also lattice vectors are labelled as follows: for layer groups with their two-dimensional lattice by **a** and **b**, for rod groups with

Table 1.2.1.1. *Classification of layer groups*

Bold or bold underlined symbols indicate Laue groups. Bold underlined point groups are also lattice point symmetries (holohedries).

Two-dimensional Bravais system	Symbol	Three-dimensional crystal system	Crystallographic point groups	No. of layer-group types	Restrictions on conventional coordinate system	Cell parameters to be determined	Bravais lattice
Oblique	*m*	Triclinic	1, $\bar{\mathbf{1}}$	2	None	*a*, *b*, γ†	*mp*
		Monoclinic	2, *m*, ***2/m***	5	$\alpha = \beta = 90°$		
Rectangular	*o*			11	$\beta = \gamma = 90°$	*a*, *b*	*op*
		Orthorhombic	222, 2*mm*, ***mmm***	30	$\alpha = \beta = \gamma = 90°$		*oc*
Square	*t*	Tetragonal	4, $\bar{4}$, ***4/m***	16	$a = b$	*a*	*tp*
			422, 4*mm*, $\bar{4}2m$, ***4/mmm***		$\alpha = \beta = \gamma = 90°$		
Hexagonal	*h*	Trigonal	3, $\bar{\mathbf{3}}$	8	$a = b$	*a*	*hp*
			32, 3*m*, $\bar{\mathbf{3}}$***m***				
		Hexagonal	6, $\bar{6}$, ***6/m***	8	$\gamma = 120°$		
			622, 6*mm*, $\bar{6}m2$, ***6/mmm***		$\alpha = \beta = 90°$		

† This angle is conventionally taken to be non-acute, *i.e.* $\geq 90°$.

Table 1.2.1.2. *Classification of rod groups*

Bold symbols indicate Laue groups.

Three-dimensional crystal system	Crystallographic point groups	No. of rod-group types	Restrictions on conventional coordinate system
Triclinic	1, $\bar{\mathbf{1}}$	2	None
Monoclinic (inclined)	2, *m*, ***2/m***	5	$\beta = \gamma = 90°$
Monoclinic (orthogonal)		5	$\alpha = \beta = 90°$
Orthorhombic	222, 2*mm*, ***mmm***	10	$\alpha = \beta = \gamma = 90°$
Tetragonal	4, $\bar{4}$, ***4/m***	19	
	422, 4*mm*, $\bar{4}2m$, ***4/mmm***		
Trigonal	3, $\bar{\mathbf{3}}$	11	$\alpha = \beta = 90$, $\gamma = 120°$
	32, 3*m*, $\bar{\mathbf{3}}$***m***		
Hexagonal	6, $\bar{6}$, ***6/m***	23	
	622, 6*mm*, $\bar{6}m2$, ***6/mmm***		

Table 1.2.1.3. *Classification of frieze groups*

Bold symbols indicate Laue groups.

Two-dimensional crystal system	Crystallographic point groups	No. of frieze-group types	Restrictions on conventional coordinate system
Oblique	1, **2**	2	None
Rectangular	*m*, ***2mm***	5	$\gamma = 90°$

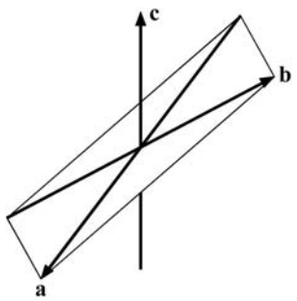

Fig. 1.2.1.1. Monoclinic/inclined basis vectors. For the monoclinic/inclined subdivision, $\beta = \gamma = 90°$ and the plane containing the **a** and **b** non-lattice basis vectors is *inclined* with respect to the lattice basis vector **c**.

their one-dimensional lattice by **c**, and for frieze groups with their one-dimensional lattice by **a**.

The selection of a crystallographic coordinate system is not unique. Following *IT* A (1983), we choose *conventional crystallographic coordinate systems* which have a right-handed set of basis vectors and such that symmetry of the subperiodic groups is best displayed. The conventional crystallographic coordinate systems used in the standard settings are given in the sixth column of Table 1.2.1.1 for the layer groups, and the fourth columns of Tables 1.2.1.2 and 1.2.1.3 for the rod groups and frieze groups, respectively. The crystallographic origin is conventionally chosen at a centre of symmetry or at a point of high site symmetry (see Section 1.2.7).

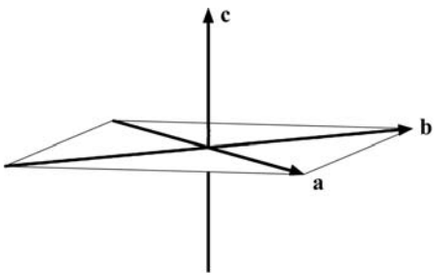

Fig. 1.2.1.2. Monoclinic/orthogonal basis vectors. For the monoclinic/orthogonal subdivision, $\alpha = \beta = 90^\circ$ and the plane containing the **a** and **b** non-lattice basis vectors is *orthogonal* to the lattice basis vector **c**.

The *conventional unit cell* of a subperiodic group is defined by the crystallographic origin and by those basis vectors which are also lattice vectors. For layer groups in the standard setting, the cell parameters, the magnitude of the lattice basis vectors **a** and **b**, and the angle between them, which specify the conventional cell, are given in the seventh column of Table 1.2.1.1. The conventional unit cell obtained in this manner turns out to be either *primitive* or *centred* and is denoted by *p* or *c*, respectively, in the eighth column of Table 1.2.1.1. For rod and frieze groups with their one-dimensional lattices, the single cell parameter to be specified is the magnitude of the lattice basis vector.

1.2.2. Contents and arrangement of the tables

The presentation of the subperiodic group tables in Parts 2, 3 and 4 follows the form and content of *IT* A (1983). The entries for a subperiodic group are printed on two facing pages or continuously on a single page, where space permits, in the following order (deviations from this standard format are indicated on the relevant pages):

Left-hand page:

(1) *Headline*;

(2) *Diagrams* for the symmetry elements and the general position;

(3) *Origin*;

(4) *Asymmetric unit*;

(5) *Symmetry operations*.

Right-hand page:

(6) *Headline* in abbreviated form;

(7) *Generators selected*: this information is the basis for the order of the entries under *Symmetry operations* and *Positions*;

(8) General and special *Positions*, with the following columns: *Multiplicity*; *Wyckoff letter*; *Site symmetry*, given by the oriented site-symmetry symbol; *Coordinates*; *Reflection conditions*;

(9) *Symmetry of special projections*;

(10) *Maximal non-isotypic non-enantiomorphic subgroups*;

(11) *Maximal isotypic subgroups and enantiomorphic subgroups of lowest index*;

(12) *Minimal non-isotypic non-enantiomorphic supergroups*.

1.2.2.1. *Subperiodic groups with more than one description*

For two monoclinic/oblique layer-group types with a glide plane, more than one description is available: *p*11*a* (L5) and *p*112/*a* (L7). The synoptic descriptions consist of abbreviated treatments for three 'cell choices', called 'cell choices 1, 2 and 3' [see Section 1.2.6, (i) *Layer groups*]. A complete description is given for cell choice 1 and it is repeated among the synoptic descriptions of cell choices 2 and 3. For three layer groups, *p*4/*n* (L52), *p*4/*nbm* (L62) and *p*4/*nmm* (L64), two descriptions are given (see Section 1.2.7). These two descriptions correspond to the choice of origin, at an inversion centre and on a fourfold axis. For 15 rod-group types, two descriptions are given, corresponding to two settings [see Section 1.2.6, (ii) *Rod groups*].

1.2.3. Headline

The description of a subperiodic group starts with a headline on a left-hand page, consisting of two or three lines which contain the following information when read from left to right.

First line:

(1) The *short international* (Hermann–Mauguin) *symbol* of the subperiodic group type. Each symbol has two meanings. The first is that of the Hermann–Mauguin symbol of the subperiodic group type. The second meaning is that of a specific subperiodic group which belongs to this subperiodic group type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 1.2.9) given on the page headed by that Hermann–Mauguin symbol, or by the given list of general positions (see Section 1.2.11). Alternatively, this group is defined by the given diagrams (see Section 1.2.6). The Hermann–Mauguin symbols for the subperiodic group types are distinct except for the rod- and frieze-group types $\not{p}1$ (R1, F1), $\not{p}211$ (R3, F2) and $\not{p}11m$ (R10, F4).

(2) The *short international* (Hermann–Mauguin) *point group symbol* for the geometric class to which the subperiodic group belongs.

(3) The name used in classifying the subperiodic group types. For layer groups this is the combination crystal system/Bravais system classification given in the first two columns of Table 1.2.1.1, and for rod and frieze groups this is the crystal system classification in the first columns of Tables 1.2.1.2 and 1.2.1.3, respectively.

Second line:

(4) The sequential number of the subperiodic group type.

(5) The *full international* (Hermann–Mauguin) *symbol* for the subperiodic group type.

(6) The *Patterson symmetry*.

Third line:

This line is used to indicate the cell choice in the case of layer groups *p*11*a* (L5) and *p*112/*a* (L7), the origin choice for the three layer groups *p*4/*n* (L52), *p*4/*nbm* (L62) and *p*4/*nmm* (L64), and the setting for the 15 rod groups with two distinct Hermann–Mauguin setting symbols (see Table 1.2.6.2).

1.2.4. International (Hermann–Mauguin) symbols for subperiodic groups

Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the subperiodic group.

(i) The letters for the two centring types for layer groups are the lower-case italic letter *p* for a primitive cell and the lower-case italic letter *c* for a centred cell. For rod and frieze groups there is only one centring type, the one-dimensional primitive cell, which is denoted by the lower-case script letter $\not{p}$.

(ii) The one or three entries after the centring letter refer to the one or three kinds of *symmetry directions* of the conventional crystallographic basis. Symmetry directions occur either as singular directions or as sets of symmetrically equivalent symmetry directions. Only one representative of each set is given. The sets of symmetry directions and their sequence in the Hermann–Mauguin symbol are summarized in Table 1.2.4.1.

Each position in the Hermann–Mauguin symbol contains one or two characters designating symmetry elements, axes and planes that occur for the corresponding crystallographic symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters are separated by a slash, *e.g.* the 4/*m* in $\not{p}4/mcc$ (R40). Crystallographic symmetry directions that carry no symmetry elements are denoted by the symbol '1', *e.g.* *p*3*m*1 (L69) and *p*112 (L2). If no misinterpretation is possible, entries '1' at the end of the symbol are omitted, as in *p*4 (L49) instead of *p*411. Subperiodic groups that have in addition to translations no

references