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

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