

1.2. GUIDE TO THE USE OF THE SUBPERIODIC GROUP TABLES

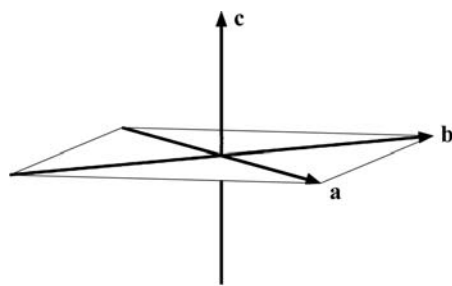


Fig. 1.2.1.2. Monoclinic/orthogonal basis vectors. For the monoclinic/orthogonal subdivision, $\alpha = \beta = 90^\circ$ and the plane containing the **a** and **b** non-lattice basis vectors is *orthogonal* to the lattice basis vector **c**.

The selection of a crystallographic coordinate system is not unique. Following *IT A* (2005), 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).

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* (2005). 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: $p11a$ (L5) and $p112/a$ (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, $p4/n$ (L52), $p4/nbm$ (L62) and $p4/nmm$ (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 $\mu 1$ (R1, F1), $\mu 211$ (R3, F2) and $\mu 11m$ (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 $p11a$ (L5) and $p112/a$ (L7), the origin choice for the three layer groups $p4/n$ (L52), $p4/nbm$ (L62) and $p4/nmm$ (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