4.1. Introduction to the synoptic tables

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4.1.1. Introduction

The synoptic tables of this section comprise two features:

(i) Space-group symbols for various settings and choices of the unit cell. Changes of the basis vectors generally cause changes of the Hermann–Mauguin space-group symbol. These axis transformations involve not only permutations of axes, conserving the shape of the cell, but also transformations which lead to different cell shapes and even to multiple cells.

(ii) Extended Hermann–Mauguin space-group symbols, in addition to the short and full symbols. The occurrence of 'additional symmetry elements' (see below) led to the introduction of 'extended space-group symbols' in *IT* (1952); they are systematically developed in the present section. These additional symmetry elements are displayed in the space-group diagrams and are important for the tabulated '*Symmetry operations*'.

For each crystal system, the text starts with a historical note on the synoptic tables in the earlier editions of *International Tables** followed by a discussion of points (i) and (ii) above. Finally, those group–subgroup relations (*cf.* Section 8.3.3) are treated that can be recognized from the full and the extended Hermann–Mauguin space-group symbols. This applies mainly to the *translationengleiche* or *t* subgroups (type **I**, *cf.* Section 2.2.15) and to the *klassengleiche* or *k* subgroups of type **IIa**. For the *k* subgroups of types **IIb** and **IIc**, inspection of the synoptic Table 4.3.2.1 provides easy recognition of only those subgroups which originate from the decentring of certain multiple cells: *C* or *F* in the tetragonal system (Section 4.3.4), *R* and *H* in the trigonal and hexagonal systems (Section 4.3.5).

4.1.2. Additional symmetry elements

In space groups, 'due to periodicity', symmetry elements occur that are not recorded in the Hermann–Mauguin symbols. These *additional symmetry elements* are products of a symmetry translation T and a symmetry operation W. This product is TW and its geometrical representation is found in the space-group diagrams (*cf.* Sections 8.1.2 and 11.1.1).†

Two cases have to be distinguished:

(i) *Symmetry operations of the same nature*

The symmetry operations W and TW are of the *same nature* and only the locations of their symmetry elements differ. This occurs when the translation vector **t** is *perpendicular* to the symmetry element of W (symmetry plane or symmetry axis); it also holds when W is an *inversion* or a *rotoinversion* (see below).

Table 4.1.2.1 summarizes the symmetry elements, located at the origin, and the location of those 'additional symmetry elements' which are generated by periodicity in the *interior* of the unit cell. 'Additional' axes $\bar{3}$, 6, 6_1, 6_2, 6_3, 6_4, 6_5 do not occur. The first column of Table 4.1.2.1 specifies W, the second column the translation vector **t**, the third the location of the symmetry element of TW. The last column indicates space groups and plane groups with representative diagrams. Other orientations of the symmetry axes and symmetry planes can easily be derived from the table.

Example

Let W be a threefold rotation with Seitz symbol $(3/0, 0, 0)$ and axis along 0, 0, *z*. The product with the translation $\mathsf{T}(1, 0, 0)$, perpendicular to the axis, is $(3/1, 0, 0)$ and again is a threefold rotation, for $(3/1, 0, 0)^3 = (1/0, 0, 0)$; its location is $\frac{2}{3}, \frac{1}{3}, z$.

Table 4.1.2.1 also deals with certain powers W^p of symmetry operations W, namely with $p = 2$ for operations of order four and with $p = 2, 3, 4$ for operations of order six. These powers give rise to their own 'additional symmetry elements', as illustrated by the following list and by the example below (operations of order 2 or 3 obviously do not have to be considered).

W	4, 4_2	4_1, 4_3	$\bar{4}$	6	$\bar{6}$	$\bar{3}$	6_1	6_5	6_3	6_2	6_4
W^p	2	2_1	2	3, 2	3, *m*	3, $\bar{1}$	3_1, 2_1	3_2, 2_1	3, 2_1	3_2, 2	3_1, 2

Example

6_2 in 0, 0, *z*; the powers to be considered are

$$(6_2)^2 = 3_2; \quad (6_2)^3 = 2; \quad (6_2)^4 = (3_2)^2.$$

The axes 3_2 and 2 at 0, 0, *z* create additional symmetry elements:

$$3_2 \text{ at } \tfrac{1}{3}, \tfrac{2}{3}, z;\ \tfrac{2}{3}, \tfrac{1}{3}, z \quad \text{and} \quad 2 \text{ at } \tfrac{1}{2}, 0, z;\ 0, \tfrac{1}{2}, z;\ \tfrac{1}{2}, \tfrac{1}{2}, z.$$

If W is an inversion operation with its centre of symmetry at point *M*, the operation TW creates an additional centre at the endpoint of the translation vector $\frac{1}{2}\mathbf{t}$, drawn from *M* (*cf.* Table 4.1.2.1, where *M* is in $0, 0, 0$).

(ii) *Symmetry operations of different nature*

The symmetry operations W and TW are of a *different nature* and have different symbols, corresponding to rotation and screw axes, to mirror and glide planes, to screw axes of different nature, and to glide planes of different nature, respectively.‡

In this case, the translation vector **t** has a component *parallel* to the symmetry axis or symmetry plane of W. This parallel component determines the nature and the symbol of the additional symmetry element, whereas the normal component of **t** is responsible for its location, as explained in Section 11.1.1. If the normal component is zero, symmetry element and additional symmetry element coincide geometrically. Note that such additional symmetry elements with glide or screw components exist even in symmorphic space groups.

Integral and centring translations: In primitive lattices, only integral translations occur and Tables 4.1.2.1 and 4.1.2.2 are relevant. For centred lattices, Tables 4.1.2.1 and 4.1.2.2 remain valid for the integral translations, whereas Table 4.1.2.3 has to be considered for the centring translations, which cause further 'additional symmetry elements'.

4.1.2.1. *Integral translations*

Table 4.1.2.2 lists representative symmetry elements, corresponding to W, and their associated glide planes and screw axes, corresponding to TW. The upper part of the table contains the diagonal twofold axes and symmetry planes that appear as tertiary symmetry elements in tetragonal and cubic space groups and as

* *Comparison tables*, pp. 28–44, *IT* (1935); *Index of symbols of space groups,* pp. 542–553, *IT* (1952).

† W is represented by $(\boldsymbol{W}, \boldsymbol{w})$ where $\boldsymbol{W}$ is the matrix part, $\boldsymbol{w}$ the column part, referred to a conventional coordinate system. T is represented by $(\boldsymbol{I}, \boldsymbol{t})$ and TW by $(\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t})$.

‡ The location and nature (screw axis, glide plane) of these additional symmetry elements were listed in the space-group tables of *IT* (1935) under the heading *Weitere Symmetrieelemente*, but were suppressed in *IT* (1952).