International Tables for Crystallography (2006). Vol. A, Chapter 4.1, pp. 56–60.

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).

Table 4.1.2.1. *Location of additional symmetry element, if the translation vector* **t** *is perpendicular to the symmetry axis along* $0, 0, z$ *or to the symmetry plane in* $x, y, 0$

The symmetry centre at 0,0,0 is included. The table is restricted to integral translations (for centring translations, see Table 4.1.2.3). The symbol ⟲ indicates cyclic permutation.

Symmetry element at the origin	Translation vector **t**	Location of additional symmetry element	Representative plane and space groups (numbers)
$2, 2_1$	1,0,0 0,1,0 1,1,0	$\frac{1}{2}, 0, z$ $0, \frac{1}{2}, z$ $\frac{1}{2}, \frac{1}{2}, z$	$P2$ (3), $P2_1$ (4), $p2$ (2)
$3, 3_1, 3_2$	1,0,0 1,1,0	$\frac{2}{3}, \frac{1}{3}, z$ $\frac{1}{3}, \frac{2}{3}, z$	$P3$ (143)–$P3_2$ (145), $p3$ (13)
$4, 4_1, 4_2, 4_3$	1,0,0	$\frac{1}{2}, \frac{1}{2}, z$	$P4$ (75)–$P4_3$ (78), $p4$(10)
$6, 6_1, 6_2, 6_3, 6_4, 6_5$	–	–	$P6$ (168)–$P6_5$ (173), $p6$ (16)
m, *a*, *b*, *n*, *d*, *e*	0,0,1	$x, y, \frac{1}{2}$	*Pm* (6), *Pa*, *Pb*, *Pn* (7), *Fddd* (70), *Cmme* (67)
$\bar{1}$	1,0,0 ⟲ 1,1,0 ⟲ 1,1,1	$\frac{1}{2}, 0, 0$ ⟲ $\frac{1}{2}, \frac{1}{2}, 0$ ⟲ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$P\bar{1}$ (2)
$\bar{3}$	–	–	$P\bar{3}$ (147)
$\bar{4}$	0,1,0	$\frac{1}{2}, \frac{1}{2}, z$	$P\bar{4}$ (81)
$\bar{6}$	0,1,0 1,1,0	$\frac{1}{3}, \frac{2}{3}, z$ $\frac{2}{3}, \frac{1}{3}, z$	$P\bar{6}$ (174)

secondary symmetry elements in rhombohedral space groups (referred to rhombohedral axes). The middle part lists the twofold axes and symmetry planes that are secondary and tertiary symmetry elements in trigonal and hexagonal space groups and secondary symmetry elements in rhombohedral space groups (referred to hexagonal axes). The lower part illustrates the occurrence of threefold screw axes in rhombohedral and cubic space groups for the orientation [111].

Note that integral translations do not produce additional glide or screw components in triclinic, monoclinic and orthorhombic groups.

Example

The operation $(3/1, 0, 0)$ in a rhombohedral or cubic space group represents a screw rotation 3_1 with axis along [111]. Indeed, the third power of $(3/1, 0, 0)$ is the translation $t(1, 1, 1)$, *i.e.* the periodicity along the threefold axis. The translation $t(1, 0, 0)$ is decomposed uniquely into the screw component $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ parallel to and the location component $\frac{2}{3}, -\frac{1}{3}, -\frac{1}{3}$ perpendicular to the threefold axis. The location of the 3_1 axis is then found to be $x, x+\frac{2}{3}, x+\frac{1}{3}$, which can also be expressed as $x+\frac{1}{3}, x, x+\frac{2}{3}$ or $x+\frac{2}{3}, x+\frac{1}{3}, x$.

For 2, *m* and *c*, the locations of the symmetry elements at the origin and within the cell can be interchanged.

Example

According to Table 4.1.2.2, the *c* plane located in *x, x, z* implies an *n* plane in $x, x+\frac{1}{2}, z$. *Vice versa*, an *n* plane in *x, x, z* implies a *c* plane in $x, x+\frac{1}{2}, z$.

In the rhombohedral space groups *R*3*c* (161) and $R\bar{3}c$ (167) and in their cubic supergroups, diagonal *n* planes in *x, x, z* and, by symmetry, in *z, x, x* and *x, z, x* coexist with *c* planes in $x, x+\frac{1}{2}, z$, *a* planes in $z, x, x+\frac{1}{2}$ and *b* planes in $x+\frac{1}{2}, z, x$, respectively (*cf.* Section 4.3.5).

Note that *the symbol of a glide plane depends on the reference frame.* Thus, the above-mentioned *n* planes in the rhombohedral description become *c* planes in the hexagonal description of *R*3*c* and $R\bar{3}c$; similarly, the *a, b* and *c* planes become *n* planes; *cf.* Sections 1.3.1 and 1.4.4.

4.1.2.2. *Centring translations**

The general rules given under (i) and (ii) remain valid. In lattices *C*, *A*, *B*, *I* and *F*, a centring vector **t** with a component parallel to the symmetry element leads to an additional symmetry element of a different kind. When the centring vector **t** is perpendicular to the symmetry element or when the symmetry element is an inversion centre or a rotoinversion axis, the additional symmetry element is of the same kind.

The first part of Table 4.1.2.3 contains pairs of *symmetry planes* related by a centring translation. Each box has three or four entries, which define three or four pairs of 'associated' planes; the cell under *F* contains all the planes under *C*, *A* and *B*. Hence, their locations are not repeated under *F*. Again, the locations of the two planes can be interchanged.

Example

The product of the *C*-centring translation, *i.e.* $t(\frac{1}{2}, \frac{1}{2}, 0)$, and the reflection through a mirror plane *m*, located in 0, *y*, *z*, is a glide reflection *b* with glide plane in $\frac{1}{4}, y, z$. Similarly, *C* centring associates a glide plane *c* in 0, *y*, *z* with a glide plane *n* in $\frac{1}{4}, y, z$.

Note that the mirror plane and 'associated' glide plane coincide geometrically when the centring translation is parallel to the mirror (*i.e.* no normal component exists); see the first cell under *A*, the second under *B*, the third cell under *C*. Also, two 'associated' glide planes (*a*, *b*) or (*b*, *c*) or (*a*, *c*) coincide geometrically. These 'double' glide planes are symbolized by '*e*'; see Table 4.1.2.3 and Section 1.3.2, Note (x).

* For the '*R* centring' see Section 4.3.5.

Table 4.1.2.2. *Additional symmetry elements and their locations, if the translation vector* **t** *is inclined to the symmetry axis or symmetry plane*

The table is restricted to integral translations and thus is valid for *P* lattices and for integral translations in centred lattices (for centring translations see Table 4.1.2.3).

Symmetry element at the origin			Additional symmetry element			Representative plane and space groups (numbers)
Symbol	Location	Translation vector **t**	Symbol	Screw or glide component	Location	
Tetragonal, rhombohedral and cubic coordinate systems						
2	$x, x, 0$	1, 0, 0 0, 1, 0	2_1	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, 0$	*P*422 (89) *R*32 (155) *P*432 (207)
m	x, x, z	1, 0, 0 0, 1, 0	*g*	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, z$	*p*4*mm* (11) *P*4*mm* (99) *R*3*m* (160) *P*$\bar{4}$3*m* (215)
c	x, x, z	1, 0, 0 0, 1, 0	*n*	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x, x+\frac{1}{2}, z$	*P*$\bar{4}$2*c* (112) *R*3*c* (161) *P*$\bar{4}$3*n* (218)
Hexagonal coordinate system						
2	$x, 0, 0$	1, 1, 0 0, 1, 0	2_1	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, 0$	*P*321 (150) *R*32 (155)
2	$x, 2x, 0$	0, 1, 0 1, 1, 0	2_1	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, 0$	*P*312 (149) *P*622 (177)
m	$x, 2x, z$	0, 1, 0 1, 1, 0	*b*	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, z$	*P*3*m*1 (156) *p*3*m*1 (14) *R*3*m* (160)
c	$x, 2x, z$	0, 1, 0 1, 1, 0	*n*	$\frac{1}{2}, 1, \frac{1}{2}$	$x, 2x+\frac{1}{2}, z$	*P*3*c*1 (158) *P*$\bar{6}$*c*2 (188) *R*3*c* (161)
m	$x, 0, z$	1, 1, 0 0, 1, 0	*a*	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, z$	*P*31*m* (157) *p*31*m* (15)
c	$x, 0, z$	1, 1, 0 0, 1, 0	*n*	$\frac{1}{2}, 0, \frac{1}{2}$ $-\frac{1}{2}, 0, \frac{1}{2}$	$x, \frac{1}{2}, z$	*P*31*c* (159) *P*$\bar{6}$2*c* (190)
Rhombohedral and cubic coordinate systems						
3	x, x, x	1, 0, 0 0, 1, 0 0, 0, 1	3_1	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	$x, x+\frac{2}{3}, x+\frac{1}{3}$	*R*3 (146) *P*23 (195)
3	x, x, x	2, 0, 0 0, 2, 0 0, 0, 2	3_2	$\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$	$x, x+\frac{1}{3}, x+\frac{2}{3}$	

Glide reflections whose square is a pure centring translation are called *d*; other diagonal glide planes are called *g* and *n*; in each case, the glide component is given between parentheses (*cf.* Sections 2.2.9 and 11.1.2).

The second part of Table 4.1.2.3 summarizes pairs of *symmetry axes* and, in the bottom line, pairs of *symmetry centres* related by a centring translation. For instance, the *B*-centring translation $t(\frac{1}{2}, 0, \frac{1}{2})$ associates a rotation axis 2 along *x*, 0, 0 with a screw axis 2_1 along $x, 0, \frac{1}{4}$. Here, too, the locations can be interchanged.

Example

The product of the translation $t(0, \frac{1}{2}, \frac{1}{2})$ with a twofold rotation around *x*, *x*, 0 is the operation $(2/0, \frac{1}{2}, \frac{1}{2})$, which occurs, for instance, in *F*432 (209). The square of this operation is the fractional translation $t(\frac{1}{2}, \frac{1}{2}, 0)$. The translation $t(0, \frac{1}{2}, \frac{1}{2})$ is decomposed into a 'screw part' $\frac{1}{4}, \frac{1}{4}, 0$ and a 'location part' $-\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$ perpendicular to it. The location of the additional symmetry element 2_1 is then found to be $x, x+\frac{1}{4}, \frac{1}{4}$ which is parallel to that of the axis 2 in *x*, *x*, 0.

Table 4.1.2.3. *Additional symmetry elements due to a centring vector* **t** *and their locations*

Symmetry element at the origin		Additional symmetry elements									Representative space groups (numbers)
		$C, t(\frac{1}{2}, \frac{1}{2}, 0)$		$A, t(0, \frac{1}{2}, \frac{1}{2})$		$B, t(\frac{1}{2}, 0, \frac{1}{2})$		$I, t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		F	
Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	
m	$0, y, z$	b	$\frac{1}{4}, y, z$	n	$0, y, z$	c	$\frac{1}{4}, y, z$	n	$\frac{1}{4}, y, z$	b, n, c, e	*Cmmm*, *Ammm*, *Bmmm* (65)
c		n		b		m		b			*Immm* (71), *Fmmm* (69)
b		m		c		n		c			*Cccm*, *Amaa*, *Bbmb* (66) *Ibca* (73)
e				e							*Aem*2 (39)
$d(0, \frac{1}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{3}{4})$		$d(0, \frac{1}{4}, \frac{3}{4})$				d, d, d	*Fddd* (70)
m	$x, 0, z$	a	$x, \frac{1}{4}, z$	c	$x, \frac{1}{4}, z$	n	$x, 0, z$	n	$x, \frac{1}{4}, z$	a, c, n, e	As above
a		m		n		c		c			
c		n		m		a		a			
e						e					*Fmm*2 (42)
$d(\frac{1}{4}, 0, \frac{1}{4})$		$d(\frac{3}{4}, 0, \frac{1}{4})$		$d(\frac{1}{4}, 0, \frac{3}{4})$		$d(\frac{3}{4}, 0, \frac{3}{4})$				d, d, d	
m	$x, y, 0$	n	$x, y, 0$	b	$x, y, \frac{1}{4}$	a	$x, y, \frac{1}{4}$	n	$x, y, \frac{1}{4}$	n, b, a, e	As above
b		a		m		n		a			
a		b		n		m		b			
e		e									*Cmme* (67)
$d(\frac{1}{4}, \frac{1}{4}, 0)$		$d(\frac{3}{4}, \frac{3}{4}, 0)$		$d(\frac{1}{4}, \frac{3}{4}, 0)$		$d(\frac{3}{4}, \frac{1}{4}, 0)$				d, d, d	
m	x, x, z	$g(\frac{1}{2}, \frac{1}{2}, 0)$	x, x, z	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x+\frac{1}{4}, z$	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x-\frac{1}{4}, z$	$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	x, x, z	g, g, g	*I*4*mm* (107), $F\bar{4}3m$ (216)
c		$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{2}, \frac{1}{2}, 0)$		n, g, g	$F\bar{4}3c$ (219)
e								e			*I*4*cm* (108)
$d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$								$d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$			$I\bar{4}3d$ (220)
2	$x, 0, 0$	2_1	$x, \frac{1}{4}, 0$	2	$x, \frac{1}{4}, \frac{1}{4}$	2_1	$x, 0, \frac{1}{4}$	2_1	$x, \frac{1}{4}, \frac{1}{4}$	$2_1, 2, 2_1$	*C*222, *A*222, *B*222 (21)
2	$0, y, 0$	2_1	$\frac{1}{4}, y, 0$	2_1	$0, y, \frac{1}{4}$	2	$\frac{1}{4}, y, \frac{1}{4}$	2_1	$\frac{1}{4}, y, \frac{1}{4}$	$2_1, 2_1, 2$	*I*222 (23)
2	$0, 0, z$	2	$\frac{1}{4}, \frac{1}{4}, z$	2_1	$0, \frac{1}{4}, z$	2_1	$\frac{1}{4}, 0, z$	2_1	$\frac{1}{4}, \frac{1}{4}, z$	$2, 2_1, 2_1$	*F*222 (22)
2	$x, \bar{x}, 0$	2	$x, \bar{x}+\frac{1}{2}, 0$	$2_1(-\frac{1}{4}, \frac{1}{4}, 0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	$2_1(\frac{1}{4}, -\frac{1}{4}, 0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	2	$x, \bar{x}, \frac{1}{4}$	$2, 2_1, 2_1$	*C*422 (*P*422) (89), *I*422 (97)
4	$0, 0, z$	4	$0, \frac{1}{2}, z$	4_2	$-\frac{1}{4}, \frac{1}{4}, z$	4_2	$\frac{1}{4}, \frac{1}{4}, z$	4_2	$0, \frac{1}{2}, z$	$4, 4_2, 4_2$	*F*432 (209)
4_1	$0, 0, z$	4_1	$0, \frac{1}{2}, z$	4_3	$-\frac{1}{4}, \frac{1}{4}, z$	4_3	$\frac{1}{4}, \frac{1}{4}, z$	4_3	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	$F4_132$ (210)
$\bar{1}$	$0, 0, 0$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{1}, \bar{1}, \bar{1}$	*Immm* (71), *Fmmm* (69)

Inversions. The 'midpoint rule' given under (i) for integral translations remains valid. When M occupies successively the eight positions of inversion centres in the primitive cell (*cf.* Table 4.1.2.1), each of the centrings *C, A, B* and *I* creates eight supplementary centres, whereas the *F* centring produces $3 \times 8 = 24$ supplementary centres, leading to a total of 32 inversion centres.

Example

For *C* centring, add $\frac{1}{4}, \frac{1}{4}, 0$ (*cf.* Table 4.1.2.3) to the eight locations of symmetry centres, given in Table 4.1.2.1, in order to obtain the eight additional symmetry centres $\frac{1}{4}, \frac{1}{4}, 0$; $\frac{3}{4}, \frac{1}{4}, 0$; $\frac{1}{4}, \frac{3}{4}, 0$; $\frac{3}{4}, \frac{3}{4}, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{3}{4}, \frac{1}{4}, \frac{1}{2}$; $\frac{1}{4}, \frac{3}{4}, \frac{1}{2}$; $\frac{3}{4}, \frac{3}{4}, \frac{1}{2}$.

Table 4.1.2.3 contains only representative cases. For 4 and 4_1 axes, only the standard orientation [001] is given. For diagonal twofold axes, only the orientation $[\bar{1}10]$ is considered. When the locations of *all* additional symmetry elements of a chosen species are desired, it is sufficient to insert the location of one of the elements into the coordinate triplets of the general position and to remove redundancies.

Example

Insert the location $x, x+\frac{2}{3}, x+\frac{1}{3}$ of a 3_1 axis (see Table 4.1.2.2) into the general position of a cubic space group to obtain four distinct locations of 3_1 axes in *P* groups and sixteen in *F* groups.

4.1.2.3. *The priority rule*

When more than one kind of symmetry element occurs for a given symmetry direction, the question of choice arises for defining the appropriate Hermann–Mauguin symbol. This choice is made in order of descending priority:

m, *e*, *a*, *b*, *c*, *n*, *d*; and rotation axes before screw axes.

This *priority rule* is explicitly stated in *IT* (1952), pages 55 and 543. It is applied to the space-group symbols in *IT* (1952) and the present edition. There are a few exceptions, however:

(i) For glide planes in *centred monoclinic* space groups, the priority rule is purposely not followed in this volume, in order to bring out the relations between the three 'cell choices' given for each setting (*cf.* Sections 2.2.16 and 4.3.2).

(ii) For *orthorhombic* space groups, the priority rule is applied only to the 'standard symbol'. The symbols for the other five settings are obtained from the standard symbol by the appropriate transformations, without invoking the priority rule again (*cf.* Table 4.3.2.1).

(iii) Space groups $I222$ (23) and $I2_12_12_1$ (24) are two distinct groups. Both contain parallel twofold rotation and screw axes and thus would receive the same symbol according to the priority rule. In $I222$, the three rotation axes and the three screw axes intersect, whereas in $I2_12_12_1$ neither the three rotation axes nor the three screw axes intersect (*cf.* Section 4.3.3).

(iv) For space group No. 73, the standard symbol *Ibca* was adopted, instead of *Ibaa* according to the rule, because *Ibca* displays the equivalence of the three symmetry directions clearly.

(v) The full symbols of space groups *Ibca* (73) and *Imma* (74) were written $I2/b\ 2/c\ 2/a$ and $I2/m\ 2/m\ 2/a$ in *IT* (1952), in application of the priority rule. In the present edition, these symbols are changed to $I2_1/b\,2_1/c\,2_1/a$ and $I2_1/m\,2_1/m\,2_1/a$, because both space groups contain $I2_12_12_1$ (and not $I222$) as subgroup.

(vi) In *tetragonal* space groups with both *a* and *b* glide planes parallel to [001], the preference was given to *b*, as in *P4bm* (100).

(vii) In *cubic* space groups where tertiary symmetry planes with glide components $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$ and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ coexist, the tertiary symmetry element was called *n* in *P* groups (instead of *a*, *b* or *c*) but *c* in *F* groups, because these symmetry elements intersect the origin.

(viii) Space groups $I23$ (197) and $I2_13$ (199) are two distinct space groups. For this pair, the same arguments apply as given above for $I222$ and $I2_12_12_1$.

Examples

$Ia\bar{3}$ (206), full symbol $I2_1/a\bar{3}$, contains $I2_13$. $P2_13$ is a maximal subgroup of $P4_132$ (213) and its enantiomorph $P4_332$ (212). A more difficult example is $I\bar{4}3d$ (220) which contains $I2_13$.*

The cubic space groups of class $m\bar{3}m$ have maximal subgroups which belong to classes 432 and $\bar{4}3m$.

Examples

$F4/m\bar{3}2/c$ (226) contains $F432$ *and* $F\bar{4}3c$; $I4_1/a\bar{3}2/d$ (230) contains $I4_132$ *and* $I\bar{4}3d$.

(*b*) *Tetragonal subgroups*

In the cubic space groups of classes 432 and $\bar{4}3m$, the primary and tertiary symmetry elements are relevant for deriving maximal tetragonal subgroups.

Examples

The groups $P432$ (207), $P4_232$ (208), $P4_332$ (212) and $P4_132$ (213) have maximal tetragonal *t* subgroups of index [3]: $P422$, $P4_222, P4_32_12$ and $P4_12_12$. $I432$ (211) gives rise to $I422$ with the same cell. $F432$ (209) also gives rise to $I422$, but *via* $F422$, so that the final unit cell is $a\sqrt{2}/2, a\sqrt{2}/2, a$.

In complete analogy, the groups $P\bar{4}3m$ (215) and $P\bar{4}3n$ (218) have maximal subgroups $P\bar{4}2m$ and $P\bar{4}2c$.†

For the space groups of class $m\bar{3}m$, the full symbols are needed to recognize their tetragonal maximal subgroups of class $4/mmm$. The primary symmetry planes of the cubic space group are conserved in the primary *and* secondary symmetry elements of the tetragonal subgroup: *m*, *n* and *d* remain in the tetragonal symbol; *a* remains *a* in the primary and becomes *c* in the secondary symmetry element of the tetragonal symbol.

Example

$P4_2/n\,\bar{3}\,2/m$ (224) and $I4_1/a\,\bar{3}\,2/d$ (230) have maximal subgroups $P4_2/n\,2/n\,2/m$ and $I4_1/a\,2/c\,2/d$, respectively, $F4_1/d\,\bar{3}\,2/c$ (228) gives rise to $F4_1/d\,2/d\,2/c$, which is equivalent to $I4_1/a\,2/c\,2/d$, all of index [3].

(*c*) *Rhombohedral subgroups*‡

Here the secondary and tertiary symmetry elements of the cubic space-group symbols are relevant. For space groups of classes 23, $m\bar{3}$, 432, the maximal *R* subgroups are $R3$, $R\bar{3}$ and $R32$, respectively. For space groups of class $\bar{4}3m$, the maximal *R* subgroup is $R3m$ when the tertiary symmetry element is *m* and $R3c$ otherwise. Finally, for space groups of class $m\bar{3}m$, the maximal *R* subgroup is $R\bar{3}m$ when the tertiary symmetry element is *m* and $R\bar{3}c$ otherwise. All subgroups are of index [4].

(*d*) *Orthorhombic subgroups*

Maximal orthorhombic space groups of index [3] are easily derived from the cubic space-group symbols of classes 23 and $m\bar{3}$.‡ Thus, $P23$, $F23$, $I23$, $P2_13$, $I2_13$ (195–199) have maximal subgroups $P222$, $F222$, $I222$, $P2_12_12_1$, $I2_12_12_1$, respectively. Likewise, maximal subgroups of $Pm\bar{3}$, $Pn\bar{3}$, $Fm\bar{3}$, $Fd\bar{3}$, $Im\bar{3}$, $Pa\bar{3}$, $Ia\bar{3}$ (200–206) are *Pmmm*, *Pnnn*, *Fmmm*, *Fddd*, *Immm*, *Pbca*, *Ibca*, respectively. The lattice type (*P*, *F*, *I*) is conserved and only the primary symmetry element has to be considered.

* From the product rule it follows that $\bar{4}$ and *d* have the same translation component so that $(\bar{4})^2 = 2_1$.

† The tertiary cubic symmetry element *n* becomes *c* in tetragonal notation.

‡ They have already been given in *IT* (1935).

References

4.1

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Revised edition: Ann Arbor: Edwards (1944). Abbreviated as *IT* (1935).]

International Tables for X-ray Crystallography (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Abbreviated as *IT* (1952).]

4.2

International Tables for X-ray Crystallography (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Abbreviated as *IT* (1952).]

4.3

Bertaut, E. F. (1976). *Study of principal subgroups and of their general positions in C and I groups of class mmm–D_{2h}. Acta Cryst.* A**32**, 380–387.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). 1. Band, edited by C. Hermann. Berlin: Borntraeger. [Revised edition: Ann Arbor: Edwards (1944). Abbreviated as IT (1935).]

International Tables for Crystallography (1995). Vol. A, fourth, revised ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers. [Abbreviated as *IT* (1995).]

International Tables for X-ray Crystallography (1952). Vol. I, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press. [Abbreviated as *IT* (1952).]

references