2.1.3.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *Site symmetry*[3] of that position. The site-symmetry group is isomorphic to a (proper or improper) subgroup of the point group to which the space group under consideration belongs. The site-symmetry groups of the different points of the same special position are conjugate (symmetry-equivalent) subgroups of the space group. For this reason, all points of one special position are described by the same site-symmetry symbol. (See Section 1.4.4 for a detailed discussion of site-symmetry groups.)

Oriented site-symmetry symbols (*cf.* Fischer *et al.*, 1973) are employed to show how the symmetry elements at a site are related to the symmetry elements of the crystal lattice. The site-symmetry symbols display the same sequence of symmetry directions as the space-group symbol (*cf.* Table 2.1.3.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. In this way, the orientation of the symmetry elements at the site is emphasized, as illustrated by the following examples.

Examples

(1) In the tetragonal space group $P4_22_12$ (94), Wyckoff position 4*f* has site symmetry ..2 and position 2*b* has site symmetry 2.22. The easiest way to interpret the symbols is to look at the dots first. For position 4*f*, the 2 is preceded by two dots and thus must belong to a tertiary symmetry direction. Only one tertiary direction is used. Consequently, the site symmetry is the monoclinic point group 2 with one of the two tetragonal tertiary directions as twofold axis.
Position *b* has one dot, with one symmetry symbol before and two symmetry symbols after it. The dot corresponds, therefore, to the secondary symmetry directions. The first symbol 2 indicates a twofold axis along the primary symmetry direction (*c* axis). The final symbols 22 indicate two twofold axes along the two mutually perpendicular tertiary directions $[1\bar{1}0]$ and [110]. The site symmetry is thus orthorhombic, 222.

(2) In the cubic space group *I*23 (197), position 6*b* has 222.. as its oriented site-symmetry symbol. The orthorhombic group 222 is completely related to the primary set of cubic symmetry directions, with the three twofold axes parallel to the three equivalent primary directions [100], [010], [001].

(3) In the cubic space group $Pn\bar{3}n$ (222), position 6*b* has 42.2 as its site-symmetry symbol. This 'cubic' site-symmetry symbol displays a tetragonal site symmetry. The position of the dot indicates that there is no symmetry along the four secondary cubic directions. The fourfold axis is connected with one of the three primary cubic symmetry directions and two equivalent twofold axes occur along the remaining two primary directions. Moreover, the group contains two mutually perpendicular (equivalent) twofold axes along those two of the six tertiary cubic directions ⟨110⟩ that are normal to the fourfold axis. Each pair of equivalent twofold axes is given by just one symbol 2. (Note that at the six sites of position 6*b* the fourfold axes are twice oriented along *a*, twice along *b* and twice along *c*.)

(4) In the tetragonal space group $P4_2/nnm$ (134), position 2*a* has site symmetry $\bar{4}2m$. The site has symmetry for all symmetry directions. Because of the presence of the primary $\bar{4}$ axis, only one of the twofold axes along the two secondary directions need be given explicitly and similarly for the mirror planes *m* perpendicular to the two tertiary directions.

The above examples show:

(i) The oriented site-symmetry symbols become identical to Hermann–Mauguin point-group symbols if the dots are omitted.

(ii) Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system than the space group under consideration.

To show, for the same type of site symmetry, how the oriented site-symmetry symbol depends on the space group under discussion, the site-symmetry group *mm*2 will be considered in orthorhombic and tetragonal space groups. Relevant crystal classes are *mm*2, *mmm*, 4*mm*, $\bar{4}2m$ and $4/mmm$. The site symmetry *mm*2 contains two mutually perpendicular mirror planes intersecting in a twofold axis.

For space groups of crystal class *mm*2, the twofold axis at the site must be parallel to the one direction of the rotation axes of the space group. The site-symmetry group *mm*2, therefore, occurs only in the orientation *mm*2. For space groups of class *mmm* (full symbol $2/m\ 2/m\ 2/m$), the twofold axis at the site may be parallel to *a*, *b* or *c* and the possible orientations of the site symmetry are 2*mm*, *m*2*m* and *mm*2. For space groups of the tetragonal crystal class 4*mm*, the twofold axis of the site-symmetry group *mm*2 must be parallel to the fourfold axis of the crystal. The two mirror planes must belong either to the two secondary or to the two tertiary tetragonal directions so that 2*mm*. and 2.*mm* are possible site-symmetry symbols. Similar considerations apply to class $\bar{4}2m$, which can occur in two settings, $\bar{4}2m$ and $\bar{4}m2$. Finally, for class $4/mmm$ (full symbol $4/m\ 2/m\ 2/m$), the twofold axis of 2*mm* may belong to any of the three kinds of symmetry directions and possible oriented site symmetries are 2*mm*., 2.*mm*, *m*2*m*. and *m*.2*m*. In the first two symbols, the twofold axis extends along the single primary direction and the mirror planes occupy either both secondary or both tertiary directions; in the last two cases, one mirror plane belongs to the primary direction and the second to either one secondary or one tertiary direction (the other equivalent direction in each case being occupied by the twofold axis).

2.1.3.13. Reflection conditions

The *Reflection conditions*[4] are listed in the right-hand column of each Wyckoff position.

These conditions are formulated here, in accordance with general practice, as 'conditions of occurrence' (structure factor not systematically zero) and not as 'extinctions' or 'systematic absences' (structure factor zero). Reflection conditions are listed for *all* those three-, two- and one-dimensional sets of reflections for which extinctions exist; hence, for those nets or rows that are *not* listed, no reflection conditions apply. The theoretical background of reflection conditions and their derivation are discussed in detail in Section 1.6.3.

[3] Often called point symmetry: *Punktsymmetrie* or *Lagesymmetrie* (German): *symétrie ponctuelle* (French).

[4] The reflection conditions were called *Auslöschungen* (German), missing spectra (English) and *extinctions* (French) in *IT* (1935) and 'Conditions limiting possible reflections' in *IT* (1952); they are often referred to as 'Systematic or space-group absences' (*cf.* Section 3.3.3).

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There are two types of systematic reflection conditions for diffraction of radiation by crystals:

(1) *General conditions*. They are associated with systematic absences caused by the presence of lattice centrings, screw axes and glide planes. The general conditions are always obeyed, irrespective of which Wyckoff positions are occupied by atoms in a particular crystal structure.
(2) *Special conditions* ('extra' conditions). They apply only to *special* Wyckoff positions and always occur in addition to the general conditions of the space group. Note that each extra condition is valid only for the scattering contribution of those atoms that are located in the relevant special Wyckoff position. If the special position is occupied by atoms whose scattering power is high in comparison with the other atoms in the structure, reflections violating the extra condition will be weak. One should note that the special conditions apply only to isotropic and spherical atoms (*cf.* Section 1.6.3).

General reflection conditions. These are due to one of three effects:

(i) *Centred cells*. The resulting conditions apply to the whole three-dimensional set of reflections *hkl*. Accordingly, they are called *integral reflection conditions*. They are given in Table 2.1.3.6. These conditions result from the centring vectors of centred cells. They disappear if a primitive cell is chosen instead of a centred cell. Note that the centring symbol and the corresponding integral reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $C \rightarrow A \rightarrow I$).
(ii) *Glide planes*. The resulting conditions apply only to two-dimensional sets of reflections, *i.e.* to reciprocal-lattice nets containing the origin (such as *hk*0, *h*0*l*, 0*kl, hhl*). For this reason, they are called *zonal reflection conditions*. The indices *hkl* of these 'zonal reflections' obey the relation $hu + kv + lw = 0$, where $[uvw]$, the direction of the zone axis, is normal to the reciprocal-lattice net. Note that the symbol of a glide plane and the corresponding zonal reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $c \rightarrow n \rightarrow a$).
(iii) *Screw axes*. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as *h*00, 0*k*0, 00*l*). They are called *serial reflection conditions*. It is interesting to note that some diagonal screw axes do not give rise to systematic absences (*cf.* Section 1.6.3 for more details).

Reflection conditions of types (ii) and (iii) are listed in Table 2.1.3.7. They can be understood as follows: Zonal and serial reflections form two- or one-dimensional sections through the origin of reciprocal space. In direct space, they correspond to projections of a crystal structure onto a plane or onto a line. Glide planes or screw axes may reduce the translation periods in these projections (*cf.* Section 2.1.3.14) and thus decrease the size of the projected cell. As a consequence, the cells in the corresponding reciprocal-lattice sections are increased, which means that systematic absences of reflections occur.

For the two-dimensional groups, the reasoning is analogous. The reflection conditions for the plane groups are assembled in Table 2.1.3.8.

For the *interpretation of observed reflections*, the general reflection conditions must be studied in the order (i) to (iii), as conditions of type (ii) may be included in those of type (i), while conditions of type (iii) may be included in those of types (i) or (ii). This is shown in the example below.

Table 2.1.3.6
Integral reflection conditions for centred cells (lattices)

Reflection condition	Centring type of cell	Centring symbol
None	Primitive	P
		R† (rhombohedral axes)
$h + k = 2n$	C-face centred	C
$k + l = 2n$	A-face centred	A
$h + l = 2n$	B-face centred	B
$h + k + l = 2n$	Body centred	I
$h + k$, $h + l$ and $k + l = 2n$ or: h, k, l all odd or all even ('unmixed')	All-face centred	F
$-h + k + l = 3n$	Rhombohedrally centred, obverse setting (standard)	R† (hexagonal axes)
$h - k + l = 3n$	Rhombohedrally centred, reverse setting	R† (hexagonal axes)
$h - k = 3n$	Hexagonally centred	H‡

† For further explanations see Section 2.1.1 and Table 2.1.1.2.
‡ For the use of the unconventional H cell, see Section 1.5.4 and Table 2.1.1.2.

In the *space-group tables*, the reflection conditions are given according to the following rules:

(i) for a given space group, all reflection conditions [up to symmetry equivalence, *cf.* rule (v)] are listed; hence for those nets or rows that are *not* listed no conditions apply. No distinction is made between 'independent' and 'included' conditions, as was done in *IT* (1952), where 'included' conditions were placed in parentheses;
(ii) the integral condition, if present, is always listed first, followed by the zonal and serial conditions;
(iii) conditions that have to be satisfied simultaneously are separated by a comma or by 'AND'. Thus, if two indices must be even, say h and l, the condition is written $h, l = 2n$ rather than $h = 2n$ and $l = 2n$. The same applies to sums of indices. Thus, there are several different ways to express the integral conditions for an F-centred lattice: '$h + k, h + l, k + l = 2n$' or '$h + k, h + l = 2n$ and $k + l = 2n$' or '$h + k = 2n$ and $h + l, k + l = 2n$' (*cf.* Table 2.1.3.6);
(iv) conditions separated by 'OR' are alternative conditions. For example, '*hkl*: $h = 2n + 1$ or $h + k + l = 4n$' means that *hkl* is 'present' if either the condition $h = 2n + 1$ *or* the alternative condition $h + k + l = 4n$ is fulfilled. Obviously, *hkl* is also a 'present' reflection if both conditions are satisfied. Note that 'or' conditions occur only for the *special conditions* described below;
(v) in crystal systems with two or more symmetry-equivalent nets or rows (tetragonal and higher), only *one* representative set (the first one in Table 2.1.3.7) is listed; *e.g.* tetragonal: only the first members of the equivalent sets 0*kl* and *h*0*l* or *h*00 and 0*k*0 are listed;
(vi) for cubic space groups, it is stated that the indices *hkl* are 'cyclically permutable' or 'permutable'. The cyclic permutability of h, k and l in all rhombohedral space groups, described with 'rhombohedral axes', and of h and k in some tetragonal space groups are not stated;

Table 2.1.3.7
Zonal and serial reflection conditions for glide planes and screw axes (*cf.* Table 2.1.2.1)

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane: Orientation of plane	Glide plane: Glide vector	Glide plane: Symbol	Crystallographic coordinate system to which condition applies	
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (a unique), Tetragonal	Orthorhombic, Cubic
	$l = 2n$		$\mathbf{c}/2$	c		
	$k + l = 2n$		$\mathbf{b}/2 + \mathbf{c}/2$	n		
	$k + l = 4n$ $(k, l = 2n)$ †		$\mathbf{b}/4 \pm \mathbf{c}/4$	d		
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (b unique), Tetragonal	Orthorhombic, Cubic
	$h = 2n$		$\mathbf{a}/2$	a		
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n		
	$l + h = 4n$ $(l, h = 2n)$ †		$\mathbf{c}/4 \pm \mathbf{a}/4$	d		
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (c unique), Tetragonal	Orthorhombic, Cubic
	$k = 2n$		$\mathbf{b}/2$	b		
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n		
	$h + k = 4n$ $(h, k = 2n)$ †		$\mathbf{a}/4 \pm \mathbf{b}/4$	d		
$h\bar{h}0l$ $0k\bar{k}l$ $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ } $\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal	
$hh.\overline{2h}.l$ $\overline{2h}.hhl$ $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$ $(01\bar{1}0)$ $(\bar{1}010)$ } $\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal	
hhl	$l = 2n$	$(1\bar{1}0)$ } $\{1\bar{1}0\}$	$\mathbf{c}/2$	c, n	Rhombohedral‡	
hkk	$h = 2n$	$(01\bar{1})$	$\mathbf{a}/2$	a, n		
hkh	$k = 2n$	$(\bar{1}01)$	$\mathbf{b}/2$	b, n		
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	c, n	Tetragonal§	Cubic¶
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1}), (011)$	$\mathbf{a}/2$	a, n		
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01), (101)$	$\mathbf{b}/2$	b, n		
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d		

† Glide planes *d* with orientations (100), (010) and (001) occur only in orthorhombic and cubic *F* space groups. Combination of the integral reflection condition (*hkl:* all odd or all even) with the zonal conditions for the *d* glide planes leads to the further conditions given between parentheses.
‡ For rhombohedral space groups described with 'rhombohedral axes', the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, *c* is always used, as in $R3c$ (161) and $R\bar{3}c$ (167), because *c* glides also occur in the hexagonal description of these space groups.
§ For tetragonal *P* space groups, the two reflection conditions (*hhl* and $h\bar{h}l$ with $l = 2n$) imply interleaving of *c* and *n* glides. In the Hermann–Mauguin space-group symbols, *c* is always used, irrespective of which glide planes contain the origin: *cf.* $P4cc$ (103), $P\bar{4}2c$ (112) and $P4/nnc$ (126).
¶ For cubic space groups, the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, either *c* or *n* is used, depending upon which glide plane contains the origin, *cf.* $P\bar{4}3n$ (218), $Pn\bar{3}n$ (222), $Pm\bar{3}n$ (223) *versus* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(vii) in the 'hexagonal-axes' descriptions of trigonal and hexagonal space groups, Bravais–Miller indices *hkil* are used. They obey two conditions:

(*a*) $h + k + i = 0$, *i.e.* $i = -(h + k)$;
(*b*) the indices h, k, i are cyclically permutable; this is not stated. Further details can be found in textbooks of crystallography.

Note that the integral reflection conditions for a rhombohedral lattice, described with 'hexagonal axes', permit the presence of only one member of the pair *hkil* and $\bar{h}\bar{k}\bar{i}l$ for $l \neq 3n$ (*cf.* Table 2.1.3.6). This applies also to the zonal reflections $h\bar{h}0l$ and $\bar{h}h0l$, which for the rhombohedral space groups must be considered separately.

Example

For a monoclinic crystal (*b* unique), the following reflection conditions have been observed:

(1) hkl: $h + k = 2n$;
(2) $0kl$: $k = 2n$; $h0l$: $h, l = 2n$; $hk0$: $h + k = 2n$;
(3) $h00$: $h = 2n$; $0k0$: $k = 2n$; $00l$: $l = 2n$.

Line (1) states that the cell used for the description of the space group is *C* centred. In line (2), the conditions $0kl$ with $k = 2n$, $h0l$ with $h = 2n$ and $hk0$ with $h + k = 2n$ are a consequence of the integral condition (1), leaving only $h0l$ with $l = 2n$ as a new condition. This indicates a glide plane *c*. Line (3) presents no new condition, since $h00$ with $h = 2n$ and $0k0$ with $k = 2n$ follow from the integral condition (1), whereas $00l$

Table 2.1.3.7 (continued)

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
*h*00	$h = 2n$	[100]	**a**/2	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$h = 4n$		**a**/4	$4_1, 4_3$	
0*k*0	$k = 2n$	[010]	**b**/2	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$k = 4n$		**b**/4	$4_1, 4_3$	
00*l*	$l = 2n$	[001]	**c**/2	2_1	Monoclinic (*c* unique), Orthorhombic; Tetragonal; Cubic
				4_2	
	$l = 4n$		**c**/4	$4_1, 4_3$	
000*l*	$l = 2n$	[001]	**c**/2	6_3	Hexagonal
	$l = 3n$		**c**/3	$3_1, 3_2, 6_2, 6_4$	
	$l = 6n$		**c**/6	$6_1, 6_5$	

with $l = 2n$ is a consequence of a zonal condition (2). Accordingly, there need not be a twofold screw axis along [010]. Space groups obeying the conditions are *Cc* (9, *b* unique, cell choice 1) and *C*2/*c* (15, *b* unique, cell choice 1). Under certain conditions, using methods based on resonant scattering, it is possible to determine whether the structure space group is centrosymmetric or not (*cf.* Section 1.6.5.1).

For a different choice of the basis vectors, the reflection conditions would appear in a different form owing to the transformation of the reflection indices (*cf.* cell choices 2 and 3 for space groups *Cc* and *C*2/*c* in Chapter 2.3). The transformations of reflection conditions under coordinate transformations are discussed and illustrated in Sections 1.5.2 and 1.5.3.

Special or 'extra' reflection conditions. These apply either to the integral reflections *hkl* or to particular sets of zonal or serial reflections. In the space-group tables, the minimal special conditions are listed that, on combination with the general conditions, are sufficient to generate the complete set of conditions. This will be apparent from the examples below.

Examples

(1) $P4_222$ (93)

General position 8*p*: 00*l*: $l = 2n$, due to 4_2; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

Special position 4*i*: *hkl*: $h + k + l = 2n$; any set of symmetry-equivalent atoms in this position displays additional *I* centring.

Special position 4*n*: 0*kl*: $l = 2n$; any set of equivalent atoms in this position displays a glide plane $c \perp [100]$. Projection of this set along [100] results in a halving of the original *c* axis, hence the special condition. Analogously for *h*0*l*: $l = 2n$.

(2) *C*12/*c*1 (15, unique axis *b*, cell choice 1)

General position 8*f*: *hkl*: $h + k = 2n$, due to the *C*-centred cell.

Special position 4*d*: *hkl*: $k + l = 2n$, due to additional *A* and *B* centring for atoms in this position. Combination with the general condition results in *hkl*: $h + k, h + l$, $k + l = 2n$ or *hkl* all odd or all even; this corresponds to an *F*-centred arrangement of atoms in this position.

Special position 4*b*: *hkl*: $l = 2n$, due to additional halving of the *c* axis for atoms in this position. Combination with the general condition results in *hkl*: $h + k, l = 2n$; this corresponds to a *C*-centred arrangement in a cell with half the original *c* axis. No further condition results from the combination.

(3) *I*12/*a*1 (15, unique axis *b*, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.1.3.15 and the space-group tables), the reflection conditions appear as follows:

General position 8*f*: *hkl*: $h + k + l = 2n$, due to the *I*-centred cell.

Special position 4*b*: *hkl*: $h = 2n$, due to additional halving of the *a* axis. Combination gives *hkl*: $h, k + l = 2n$, *i.e.* an *A*-centred arrangement of atoms in a cell with half the original *a* axis.

An analogous result is obtained for position 4*d*.

Table 2.1.3.8
Reflection conditions for the plane groups

Type of reflections	Reflection condition	Centring type of plane cell; or glide line with glide vector	Coordinate system to which condition applies
hk	None	Primitive *p*	All systems
	$h + k = 2n$	Centred *c*	Rectangular
	$h - k = 3n$	Hexagonally centred *h*†	Hexagonal
*h*0	$h = 2n$	Glide line *g* normal to *b* axis; glide vector $\frac{1}{2}\mathbf{a}$	Rectangular, Square
0*k*	$k = 2n$	Glide line *g* normal to *a* axis; glide vector $\frac{1}{2}\mathbf{b}$	

† For the use of the unconventional *h* cell see Table 2.1.1.2.

(4) *Fmm*2 (42)

General position 16*e*: *hkl*: $h + k, h + l, k + l = 2n$, due to the *F*-centred cell.

Special position 8*b*: *hkl*: $= 2n$, due to additional halving of the *a* axis. Combination results in *hkl*: $h, k, l = 2n$, *i.e.* all indices even; the atoms in this position are arranged in a primitive lattice with axes $\frac{1}{2}a$, $\frac{1}{2}b$ and $\frac{1}{2}c$.

For the cases where the special reflection conditions are described by means of combinations of 'OR' and 'AND' instructions, the 'AND' condition always has to be evaluated with priority, as shown by the following example.

Example: P$\bar{4}$3*n (218)*

Special position 6*d*: *hkl*: $h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$.

This expression contains the following two conditions:

(*a*) *hkl*: $h + k + l = 2n$;

(*b*) $h = 2n + 1$ and $k = 4n$ and $l = 4n + 2$.

A reflection is 'present' (occurring) if either condition (*a*) is satisfied or if a permutation of the three conditions in (*b*) are simultaneously fulfilled.

Structural or non-space-group absences. Note that in addition *non-space-group absences* may occur that are not due to the symmetry of the space group (*i.e.* centred cells, glide planes or screw axes). Atoms in general or special positions may cause additional systematic absences if their coordinates assume special values [*e.g.* 'noncharacteristic orbits'; *cf.* Section 1.4.4.4 and Engel *et al.* (1984)]. Non-space-group absences may also occur for special arrangements of atoms ('false symmetry') in a crystal structure (*cf.* Templeton, 1956; Sadanaga *et al.*, 1978). Non-space-group absences may occur also for polytypic structures; this is briefly discussed by Durovič in Section 9.2.2.2.5 of *International Tables for Crystallography* (2004), Vol. C. Even though all these 'structural absences' are fortuitous and due to the special arrangements of atoms in a particular crystal structure, they have the appearance of space-group absences. Occurrence of structural absences thus may lead to an *incorrect assignment of the space group*. Accordingly, the reflection conditions in the space-group tables must be considered as a minimal set of conditions.

The use of reflection conditions and of the symmetry of reflection intensities for space-group determination is described in Chapter 1.6.

2.1.3.14. Symmetry of special projections

Projections of crystal structures are used by crystallographers in special cases. Use of so-called 'two-dimensional data' (zero-layer intensities) results in the projection of a crystal structure along the normal to the reciprocal-lattice net. A detailed treatment of projections of space groups, including basic definitions and illustrative examples, is given in Section 1.4.5.3.

Even though the projection of a finite object along *any* direction may be useful, the projection of a *periodic* object such as a crystal structure is only sensible along a rational lattice direction (lattice row). Projection along a nonrational direction results in a constant density in at least one direction.

Data listed in the space-group tables. Under the heading *Symmetry of special projections*, the following data are listed for three projections of each space group; no projection data are given for the plane groups.

(i) *The projection direction*. All projections are orthogonal, *i.e.* the projection is made onto a plane normal to the projection direction. This ensures that spherical atoms appear as circles in the projection. For each space group, three projections are listed. If a lattice has three kinds of symmetry directions, the three projection directions correspond to the primary, secondary and tertiary symmetry directions of the lattice (*cf.* Table 2.1.3.1). If a lattice contains fewer than three kinds of symmetry directions, as in the triclinic, monoclinic and rhombohedral cases, the additional projection direction(s) are taken along coordinate axes, *i.e.* lattice rows lacking symmetry.

The directions for which projection data are listed are as follows:

Triclinic Monoclinic (both settings) Orthorhombic	[001]	[100]	[010]
Tetragonal	[001]	[100]	[110]
Hexagonal	[001]	[100]	[210]
Rhombohedral	[111]	[1$\bar{1}$0]	[2$\bar{1}\bar{1}$]
Cubic	[001]	[111]	[110]

(ii) *The Hermann–Mauguin symbol of the plane group* resulting from the projection of the space group. If necessary, the symbols are given in oriented form; for example, plane group *pm* is expressed either as *p*1*m*1 or as *p*11*m* (*cf.* Section 1.4.1.5 for explanations of Hermann–Mauguin symbols of plane groups).

(iii) *Relations between the basis vectors* $\mathbf{a}'$, $\mathbf{b}'$ of the plane group and the basis vectors **a**, **b**, **c** of the space group. Each set of basis vectors refers to the conventional coordinate system of the plane group or space group, as employed in Chapters 2.2 and 2.3. The basis vectors of the two-dimensional cell are always called $\mathbf{a}'$ and $\mathbf{b}'$ irrespective of which two of the basis vectors **a**, **b**, **c** of the three-dimensional cell are projected to form the plane cell. All relations between the basis vectors of the two cells are expressed as vector equations, *i.e.* $\mathbf{a}'$ and $\mathbf{b}'$ are given as linear combinations of **a**, **b** and **c**. For the triclinic or monoclinic space groups, basis vectors **a**, **b** or **c** inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$.

For primitive three-dimensional cells, the *metrical* relations between the lattice parameters of the space group and the plane group are collected in Table 2.1.3.9. The additional relations for centred cells can be derived easily from the table.

(iv) *Location of the origin* of the plane group with respect to the unit cell of the space group. The same description is used as for the location of symmetry elements (*cf.* Section 2.1.3.9).

Example

'Origin at *x*, 0, 0' or 'Origin at $\frac{1}{4}, \frac{1}{4}, z$'.

Projections of centred cells (lattices). For centred lattices, two different cases may occur:

(i) The projection direction is parallel to a lattice-centring vector. In this case, the projected plane cell is primitive for the centring types *A*, *B*, *C*, *I* and *R*. For *F*-centred lattices, the multiplicity is reduced from 4 to 2 because *c*-centred plane