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).

Table 2.2.13.1. *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	
$h-k=3n$	Hexagonally centred	H†

* For further explanations see Chapters 1.2 and 2.1.

† For the use of the unconventional *H* cell, see Chapter 1.2.

2.2.13. Reflection conditions

The *Reflection conditions** 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.

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

(1) *General conditions*. They apply to *all* Wyckoff positions of a space group, *i.e.* they 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 occur always 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.

2.2.13.1. *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 2.2.13.1. 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: $C \rightarrow A \rightarrow I$).

* 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.* Chapter 12.3).

Table 2.2.13.2. *Zonal and serial reflection conditions for glide planes and screw axes (cf. Chapter 1.3)*

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane			Crystallographic coordinate system to which condition applies
		Orientation of plane	Glide vector	Symbol	
$0kl$	$k = 2n$	(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 hkk hkh	$l = 2n$ $h = 2n$ $k = 2n$	$(1\bar{1}0)$ $(01\bar{1})$ $(\bar{1}01)$ $\}\{1\bar{1}0\}$	$\mathbf{c}/2$ $\mathbf{a}/2$ $\mathbf{b}/2$	c, n a, n b, n	Rhombohedral†
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	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, *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 occur also 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) *vs* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(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 contain-

Table 2.2.13.2. (*cont.*)

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
$h00$	$h = 2n$	[100]	$\mathbf{a}/2$	2_1	Monoclinic (a unique), Orthorhombic, Tetragonal, Cubic
				4_2	
	$h = 4n$		$\mathbf{a}/4$	$4_1, 4_3$	
$0k0$	$k = 2n$	[010]	$\mathbf{b}/2$	2_1	Monoclinic (b unique), Orthorhombic, Tetragonal, Cubic
				4_2	
	$k = 4n$		$\mathbf{b}/4$	$4_1, 4_3$	
$00l$	$l = 2n$	[001]	$\mathbf{c}/2$	2_1	Monoclinic (c unique), Orthorhombic, Cubic
				4_2	Tetragonal, Cubic
	$l = 4n$		$\mathbf{c}/4$	$4_1, 4_3$	
$000l$	$l = 2n$	[001]	$\mathbf{c}/2$	6_3	Hexagonal
	$l = 3n$		$\mathbf{c}/3$	$3_1, 3_2, 6_2, 6_4$	
	$l = 6n$		$\mathbf{c}/6$	$6_1, 6_5$	

ing the origin (such as $h00$, $0k0$, $00l$). They are called *serial reflection conditions*.

Reflection conditions of types (ii) and (iii) are listed in Table 2.2.13.2. 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 2.2.14) 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 2.2.13.3.

Table 2.2.13.3. *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
$h0$	$h = 2n$	Glide line g normal to b axis; glide vector $\frac{1}{2}\mathbf{a}$	Rectangular, Square
$0k$	$k = 2n$	Glide line g normal to a axis; glide vector $\frac{1}{2}\mathbf{b}$	

* For the use of the unconventional h cell see Chapter 1.2.

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.

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

(i) for a given space group, *all* reflection conditions 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 satisified 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 2.2.13.1);

(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 a 'present' reflection also if both conditions are satisfied. Note that 'or' conditions occur only for the *special conditions* described in Section 2.2.13.2;

(v) in crystal systems with two or more symmetrically equivalent nets or rows (tetragonal and higher), only *one* representative set (the first one in Table 2.2.13.2) is listed; *e.g.* tetragonal: only the first members of the equivalent sets $0kl$ and $h0l$ or $h00$ and $0k0$ 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;

(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 2.2.13.1). 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 $00l$ 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 $C2/c$ (15, b unique, cell choice 1). On the basis of diffraction symmetry and reflection conditions, no choice between the two space groups can be made (*cf.* Part 3).

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 $C2/c$ in Part 7).

2.2.13.2. *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 $8p$: $00l$: $l = 2n$, due to 4_2; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

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

Special position $4n$: $0kl$: $l = 2n$; 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, whence the special condition. Analogously for $h0l$: $l = 2n$.

(2) $C12/c1$ (15, unique axis b, cell choice 1)

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

Special position $4d$: 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 $4b$: 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) $I12/a1$ (15, unique axis b, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.2.16 and space-group tables), the reflection conditions appear as follows:

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

Special position $4b$: 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 $4d$.

(4) $Fmm2$ (42)

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

Special position $8b$: hkl: $h = 2n$, 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: $P\bar{4}3n$ (218)

Special position $6d$: 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.

2.2.13.3. *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' (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 Part 3.