these centring translations have to be added to the listed coordinate triplets. Note that not all points of a position always lie within the unit cell; some may be outside since the coordinates are formulated modulo 1; thus, for example, $\bar{x},\bar{y},\bar{z}$ is written rather than $\bar{x}+1,\bar{y}+1,\bar{z}+1$.

The M coordinate triplets of a position represent the coordinates of the M equivalent points (atoms) in the unit cell. A graphic representation of the points of the general position is provided by the general-position diagram; *cf.* Section 2.2.6.

(v) *Reflection conditions*. These are described in Section 2.2.13.

The two types of positions, general and special, are characterized as follows:

(i) *General position*

A set of symmetrically equivalent points, *i.e.* a 'crystallographic orbit', is said to be in 'general position' if each of its points is left invariant only by the identity operation but by no other symmetry operation of the space group. Each space group has only one general position.

The coordinate triplets of a general position (which always start with x, y, z) can also be interpreted as a short-hand form of the matrix representation of the symmetry operations of the space group; this viewpoint is further described in Sections 8.1.6 and 11.1.1.

(ii) *Special position(s)*

A set of symmetrically equivalent points is said to be in 'special position' if each of its points is mapped onto itself by the identity and at least one further symmetry operation of the space group. This implies that specific constraints are imposed on the coordinates of each point of a special position; *e.g.* $x=\frac{1}{4},y=0$, leading to the triplet $\frac{1}{4},0,z$; or $y=x+\frac{1}{2}$, leading to the triplet $x,x+\frac{1}{2},z$. The number of special positions in a space group [up to 26 in *Pmmm* (No. 47)] depends on the number and types of symmetry operations that map a point onto itself.

The set of *all* symmetry operations that map a point onto itself forms a group, known as the 'site-symmetry group' of that point. It is given in the third column by the 'oriented site-symmetry symbol' which is explained in Section 2.2.12. General positions always have site symmetry 1, whereas special positions have higher site symmetries, which can differ from one special position to another.

If in a crystal structure the centres of finite objects, such as molecules, are placed at the points of a special position, each such object must display a point symmetry that is at least as high as the site symmetry of the special position. Geometrically, this means that the centres of these objects are located on symmetry elements without translations (centre of symmetry, mirror plane, rotation axis, rotoinversion axis) or at the intersection of several symmetry elements of this kind (*cf.* space-group diagrams).

Note that the location of an object on a screw axis or on a glide plane does *not* lead to an increase in the site symmetry and to a consequent reduction of the multiplicity for that object. Accordingly, a space group that contains only symmetry elements *with* translation components does not have any special position. Such a space group is called 'fixed-point-free'. The 13 space groups of this kind are listed in Section 8.3.2.

Example: Space group $C12/c1$ (15, unique axis b, cell choice 1)

The general position 8*f* of this space group contains eight equivalent points per cell, each with site symmetry 1. The coordinate triplets of four points, (1) to (4), are given explicitly, the coordinates of the other four points are obtained by adding the components $\frac{1}{2},\frac{1}{2},0$ of the C-centring translation to the coordinate triplets (1) to ($\bar{4}$).

The space group has five special positions with Wyckoff letters *a* to *e*. The positions 4*a* to 4*d* require inversion symmetry, $\bar{1}$, whereas Wyckoff position 4*e* requires twofold rotation symmetry, 2, for any object in such a position. For position 4*e*, for instance, the four equivalent points have the coordinates $0,y,\frac{1}{4}$; $0,\bar{y},\frac{3}{4}$; $\frac{1}{2},y+\frac{1}{2},\frac{1}{4}$; $\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$. The values of x and z are specified, whereas y may take any value. Since each point of position 4*e* is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from 8 to 4, whereas the order of the site-symmetry group is increased from 1 to 2.

From the entries 'Symmetry operations', the locations of the four twofold axes can be deduced as $0,y,\frac{1}{4}$; $0,y,\frac{3}{4}$; $\frac{1}{2},y,\frac{1}{4}$; $\frac{1}{2},y,\frac{3}{4}$.

From this example, the general rule is apparent that the product of the position multiplicity and the order of the corresponding site-symmetry group is constant for all Wyckoff positions of a given space group; it is the multiplicity of the general position.

Attention is drawn to ambiguities in the description of crystal structures in a few space groups, depending on whether the coordinate triplets of *IT* (1952) or of this edition are taken. This problem is analysed by Parthé *et al.* (1988).

2.2.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *Site symmetry** 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 (symmetrically equivalent) subgroups of the space group. For this reason, all points of one special position are described by the same site-symmetry symbol.

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 2.2.4.1). 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 $I23$ (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

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

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).