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).

references