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: $C \to A \to I$).

(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 $hk0$, $h0l$, $0kl$, 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: $c \to n \to a$).

(iii) *Screw axes*. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as $h00$, $0k0$, $00l$). 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	
$h - k = 3n$	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 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 2.1.3.6);

(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 $0kl$ 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;

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