

3.22: Reflection conditions

The reflection conditions describe the conditions of occurrence of a reflection (structure factor not systematically zero). 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. They are due to one of three effects:

- *Centered 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 1.

- *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*. For instance, for a glide plane parallel to (001) :

type of reflection	reflection condition	glide vector	glide plane
$0kl$	$k = 2n$	$\mathbf{b}/2$	b
	$l = 2n$	$\mathbf{c}/2$	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

The zonal reflection conditions are listed in Table 2.2.13.2 of *International Tables of Crystallography, Volume A*.

- *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*. For instance, for a screw axis parallel to $[001]$, the reflection conditions are:

type of reflection	reflection condition	screw vector	screw axis
$00l$	$l = 2n$	$\mathbf{c}/2$	$2_1; 4_2$
	$l = 4n$	$\mathbf{c}/4$	$4_1; 4_3$
$000l$	$l = 2n$	$\mathbf{c}/2$	6_3
	$l = 3n$	$\mathbf{c}/3$	$4_1; 3_1; 3_2; 6_2; 6_4$
	$l = 6n$	$\mathbf{c}/6$	$6_1; 6_5$

The serial reflection conditions are listed in Table 2.2.13.2 of *International Tables of Crystallography, Volume A*.

(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.

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