

2.2. CONTENTS AND ARRANGEMENT OF THE TABLES

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
	$h = 4n$			$\mathbf{a}/4$	
			$4_1, 4_3$		
$0k0$	$k = 2n$	[010]	$\mathbf{b}/2$	2_1	{ Monoclinic (b unique), Orthorhombic, Tetragonal } } Cubic
	$k = 4n$			$\mathbf{b}/4$	
			$4_1, 4_3$		
$00l$	$l = 2n$	[001]	$\mathbf{c}/2$	2_1	{ Monoclinic (c unique), Orthorhombic } } Tetragonal } Cubic
	$l = 4n$			$\mathbf{c}/4$	
			$4_1, 4_3$		
$000l$	$l = 2n$	[001]	$\mathbf{c}/2$	6_3	} Hexagonal
	$l = 3n$			$3_1, 3_2, 6_2, 6_4$	
	$l = 6n$			$6_1, 6_5$	

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 satisfied 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