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Table 2.1.3.7

Zonal and serial reflection conditions for glide planes and screw axes (*cf.* Table 2.1.2.1)

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane: Orientation of plane	Glide plane: Glide vector	Glide plane: Symbol	Crystallographic coordinate system to which condition applies	
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (a unique), Tetragonal	Orthorhombic, Cubic
	$l = 2n$		$\mathbf{c}/2$	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		
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (b unique), Tetragonal	Orthorhombic, Cubic
	$h = 2n$		$\mathbf{a}/2$	a		
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n		
	$l + h = 4n$ $(l, h = 2n)$ †		$\mathbf{c}/4 \pm \mathbf{a}/4$	d		
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (c unique), Tetragonal	Orthorhombic, Cubic
	$k = 2n$		$\mathbf{b}/2$	b		
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n		
	$h + k = 4n$ $(h, k = 2n)$ †		$\mathbf{a}/4 \pm \mathbf{b}/4$	d		
$h\bar{h}0l$ $0k\bar{k}l$ $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ } $\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal	
$hh.\overline{2h}.l$ $\overline{2h}.hhl$ $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$ $(01\bar{1}0)$ $(\bar{1}010)$ } $\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal	
hhl hkk hkh	$l = 2n$ $h = 2n$ $k = 2n$	$(1\bar{1}0)$ $(01\bar{1})$ $(\bar{1}01)$ } $\{1\bar{1}0\}$	$\mathbf{c}/2$ $\mathbf{a}/2$ $\mathbf{b}/2$	c, n a, n b, n	Rhombohedral‡	
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0)$, (110)	$\mathbf{c}/2$	c, n	Tetragonal§	Cubic¶
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1})$, (011)	$\mathbf{a}/2$	a, n		
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01)$, (101)	$\mathbf{b}/2$	b, n		
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d		

† Glide planes d with orientations (100), (010) and (001) occur only in orthorhombic and cubic F space groups. Combination of the integral reflection condition (hkl: all odd or all even) with the zonal conditions for the d glide planes leads to the further conditions given between parentheses.

‡ For rhombohedral space groups described with 'rhombohedral axes', the three reflection conditions ($l = 2n$, $h = 2n$, $k = 2n$) imply interleaving of c and n glides, a and n glides, and b and n glides, respectively. In the Hermann–Mauguin space-group symbols, c is always used, as in $R3c$ (161) and $R\bar{3}c$ (167), because c glides also occur in the hexagonal description of these space groups.

§ For tetragonal P space groups, the two reflection conditions (hhl and $h\bar{h}l$ with $l = 2n$) imply interleaving of c and n glides. In the Hermann–Mauguin space-group symbols, c is always used, irrespective of which glide planes contain the origin: *cf.* $P4cc$ (103), $P\bar{4}2c$ (112) and $P4/nnc$ (126).

¶ For cubic space groups, the three reflection conditions ($l = 2n$, $h = 2n$, $k = 2n$) imply interleaving of c and n glides, a and n glides, and b and n glides, respectively. In the Hermann–Mauguin space-group symbols, either c or n is used, depending upon which glide plane contains the origin, *cf.* $P\bar{4}3n$ (218), $Pn\bar{3}n$ (222), $Pm\bar{3}n$ (223) *versus* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(vii) in the 'hexagonal-axes' descriptions of trigonal and hexagonal space groups, Bravais–Miller indices $hkil$ are used. They obey two conditions:

(*a*) $h + k + i = 0$, *i.e.* $i = -(h + k)$;

(*b*) the indices h, k, i are cyclically permutable; this is not stated. Further details can be found in textbooks of crystallography.

Note that the integral reflection conditions for a rhombohedral lattice, described with 'hexagonal axes', permit the presence of only one member of the pair $hkil$ and $\bar{h}\bar{k}\bar{i}l$ for $l \neq 3n$ (*cf.* Table 2.1.3.6). This applies also to the zonal reflections $h\bar{h}0l$ and $\bar{h}h0l$, which for the rhombohedral space groups must be considered separately.

Example

For a monoclinic crystal (b unique), the following reflection conditions have been observed:

(1) hkl: $h + k = 2n$;
(2) $0kl$: $k = 2n$; $h0l$: $h, l = 2n$; $hk0$: $h + k = 2n$;
(3) $h00$: $h = 2n$; $0k0$: $k = 2n$; $00l$: $l = 2n$.

Line (1) states that the cell used for the description of the space group is C centred. In line (2), the conditions $0kl$ with $k = 2n$, $h0l$ with $h = 2n$ and $hk0$ with $h + k = 2n$ are a consequence of the integral condition (1), leaving only $h0l$ with $l = 2n$ as a new condition. This indicates a glide plane c. Line (3) presents no new condition, since $h00$ with $h = 2n$ and $0k0$ with $k = 2n$ follow from the integral condition (1), whereas $00l$

Table 2.1.3.7 (continued)

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis: Direction of axis	Screw vector	Symbol	Crystallographic coordinate system to which condition applies
$h00$	$h = 2n$	[100]	$\mathbf{a}/2$	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal; Cubic
				4_2	Cubic
	$h = 4n$		$\mathbf{a}/4$	$4_1, 4_3$	Cubic
$0k0$	$k = 2n$	[010]	$\mathbf{b}/2$	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal; Cubic
				4_2	Cubic
	$k = 4n$		$\mathbf{b}/4$	$4_1, 4_3$	Cubic
$00l$	$l = 2n$	[001]	$\mathbf{c}/2$	2_1	Monoclinic (*c* unique), Orthorhombic; Cubic
				4_2	Tetragonal; Cubic
	$l = 4n$		$\mathbf{c}/4$	$4_1, 4_3$	Tetragonal; Cubic
$000l$	$l = 2n$	[001]	$\mathbf{c}/2$	6_3	Hexagonal
	$l = 3n$		$\mathbf{c}/3$	$3_1, 3_2, 6_2, 6_4$	Hexagonal
	$l = 6n$		$\mathbf{c}/6$	$6_1, 6_5$	Hexagonal

with $l = 2n$ is a consequence of a zonal condition (2). Accordingly, there need not be a twofold screw axis along [010]. Space groups obeying the conditions are *Cc* (9, *b* unique, cell choice 1) and $C2/c$ (15, *b* unique, cell choice 1). Under certain conditions, using methods based on resonant scattering, it is possible to determine whether the structure space group is centrosymmetric or not (*cf.* Section 1.6.5.1).

For a different choice of the basis vectors, the reflection conditions would appear in a different form owing to the transformation of the reflection indices (*cf.* cell choices 2 and 3 for space groups *Cc* and $C2/c$ in Chapter 2.3). The transformations of reflection conditions under coordinate transformations are discussed and illustrated in Sections 1.5.2 and 1.5.3.

Special or 'extra' reflection conditions. These apply either to the integral reflections *hkl* or to particular sets of zonal or serial reflections. In the space-group tables, the minimal special conditions are listed that, on combination with the general conditions, are sufficient to generate the complete set of conditions. This will be apparent from the examples below.

Examples

(1) $P4_222$ (93)

General position 8*p*: 00*l*: $l = 2n$, due to 4_2; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

Special position 4*i*: *hkl*: $h + k + l = 2n$; any set of symmetry-equivalent atoms in this position displays additional *I* centring.

Special position 4*n*: 0*kl*: $l = 2n$; any set of equivalent atoms in this position displays a glide plane $c \perp [100]$. Projection of this set along [100] results in a halving of the original *c* axis, hence the special condition. Analogously for *h*0*l*: $l = 2n$.

(2) $C12/c1$ (15, unique axis *b*, cell choice 1)

General position 8*f*: *hkl*: $h + k = 2n$, due to the *C*-centred cell.

Special position 4*d*: *hkl*: $k + l = 2n$, due to additional *A* and *B* centring for atoms in this position. Combination with the general condition results in *hkl*: $h + k, h + l, k + l = 2n$ or *hkl* all odd or all even; this corresponds to an *F*-centred arrangement of atoms in this position.

Special position 4*b*: *hkl*: $l = 2n$, due to additional halving of the *c* axis for atoms in this position. Combination with the general condition results in *hkl*: $h + k, l = 2n$; this corresponds to a *C*-centred arrangement in a cell with half the original *c* axis. No further condition results from the combination.

(3) $I12/a1$ (15, unique axis *b*, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.1.3.15 and the space-group tables), the reflection conditions appear as follows:

General position 8*f*: *hkl*: $h + k + l = 2n$, due to the *I*-centred cell.

Special position 4*b*: *hkl*: $h = 2n$, due to additional halving of the *a* axis. Combination gives *hkl*: $h, k + l = 2n$, *i.e.* an *A*-centred arrangement of atoms in a cell with half the original *a* axis.

An analogous result is obtained for position 4*d*.

Table 2.1.3.8
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
*h*0	$h = 2n$	Glide line *g* normal to *b* axis; glide vector $\frac{1}{2}\mathbf{a}$	Rectangular, Square
0*k*	$k = 2n$	Glide line *g* normal to *a* axis; glide vector $\frac{1}{2}\mathbf{b}$	Rectangular, Square

† For the use of the unconventional *h* cell see Table 2.1.1.2.