Table 1.6.3.1
Effect of lattice type on conditions for possible reflections

Lattice type	$\boldsymbol{w}_L^T$	$\mathbf{h}\boldsymbol{w}_L$	Conditions for possible reflections
P	(0, 0, 0)	Integer	None
A	$(0, \frac{1}{2}, \frac{1}{2})$	$(k+l)/2$	hkl: $k+l=2n$
B	$(\frac{1}{2}, 0, \frac{1}{2})$	$(h+l)/2$	hkl: $h+l=2n$
C	$(\frac{1}{2}, \frac{1}{2}, 0)$	$(h+k)/2$	hkl: $h+k=2n$
I	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(h+k+l)/2$	hkl: $h+k+l=2n$
F	$(0, \frac{1}{2}, \frac{1}{2})$	$(k+l)/2$	h, k and l are all even or all odd (simultaneous fulfillment of the conditions for types A, B and C).
	$(\frac{1}{2}, 0, \frac{1}{2})$	$(h+l)/2$	
	$(\frac{1}{2}, \frac{1}{2}, 0)$	$(h+k)/2$	
$R_{\rm obv}$	$(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$	$(2h+k+l)/3$	hkl: $-h+k+l=3n$
	$(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$	$(h+2k+2l)/3$	(triple hexagonal cell in obverse orientation)
$R_{\rm rev}$	$(\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$	$(h+2k+l)/3$	hkl: $h-k+l=3n$
	$(\frac{2}{3}, \frac{1}{3}, \frac{2}{3})$	$(2h+k+2l)/3$	(triple hexagonal cell in reverse orientation)

Table 1.6.3.2
Effect of some glide reflections on conditions for possible reflections

Glide reflection	$\boldsymbol{w}^T$	$\mathbf{h}$	Conditions for possible reflections
$a \perp [001]$	$(1/2, 0, z)$	$(hk0)$	$hk0$: $h=2n$
$b \perp [001]$	$(0, 1/2, z)$	$(hk0)$	$hk0$: $k=2n$
$n \perp [001]$	$(1/2, 1/2, z)$	$(hk0)$	$hk0$: $h+k=2n$
$d \perp [001]$	$(1/4, \pm 1/4, z)$	$(hk0)$	$hk0$: $h+k=4n$ $(h, k=2n)$

Table 1.6.3.3
Effect of some screw rotations on conditions for possible reflections

Screw rotation	$\boldsymbol{w}^T$	$\mathbf{h}$	Conditions for possible reflections
$2_1 \parallel [100]$	$(1/2, y, z)$	$(h00)$	$h00$: $h=2n$
$2_1 \parallel [010]$	$(x, 1/2, z)$	$(0k0)$	$0k0$: $k=2n$
$2_1 \parallel [001]$	$(x, y, 1/2)$	$(00l)$	$00l$: $l=2n$
$2_1 \parallel [110]$	$(1/2, 1/2, z)$	$(hh0)$	None
$3_1 \parallel [001]$	$(x, y, 1/3)$	$(00l)$	$00l$: $l=3n$
$3_1 \parallel [111]$	$(1/3, 1/3, 1/3)$	(hhh)	None
$4_1 \parallel [001]$	$(x, y, 1/4)$	$(00l)$	$00l$: $l=4n$
$6_1 \parallel [001]$	$(x, y, 1/6)$	$(00l)$	$00l$: $l=6n$

$k = 2n$. $0k0$ reflections with odd k will be systematically absent. A brief summary of the effects of various screw rotations on the conditions for possible reflections from the corresponding special subsets of hkl is given in Table 1.6.3.3. Note, however, that while the presence of a twofold screw axis parallel to $\mathbf{b}$ ensures the condition $0k0$: $k = 2n$, the actual observation of such a condition can be taken as an indication but not as absolute proof of the presence of a screw axis in the crystal.

It is interesting to note that some diagonal screw axes do not give rise to conditions for possible reflections. For example, let $\boldsymbol{W}$ be the matrix of a threefold rotation operation parallel to [111] and $\boldsymbol{w}^T$ be given by (1/3, 1/3, 1/3). It is easy to show that the diffraction vector that remains unchanged when postmultiplied by $\boldsymbol{W}$ has the form $\mathbf{h} = (hhh)$ and, obviously, for such $\mathbf{h}$ and $\boldsymbol{w}$, $\mathbf{h}\boldsymbol{w} = h$. Since this scalar product is an integer there are, according to equation (1.6.3.7), no values of the index h for which the structure factor $F(hhh)$ must be absent.

A short discussion of special reflection conditions

The conditions for possible reflections arising from lattice types, glide reflections and screw rotations are related to general equivalent positions and are known as *general reflection conditions*. There are also *special* or '*extra*' reflection conditions that arise from the presence of atoms in special positions. These conditions are observable if the atoms located in special positions are much heavier than the rest. The minimal special conditions are listed in the space-group tables in Chapter 2.3. They can sometimes be understood if the geometry of a given specific site is examined. For example, Wyckoff position $4i$ in space group $P4_222$ (93) can host four atoms, at coordinates

$$4i:\ 0, \tfrac{1}{2}, z;\quad \tfrac{1}{2}, 0, z+\tfrac{1}{2};\quad 0, \tfrac{1}{2}, \bar{z};\quad \tfrac{1}{2}, 0, \bar{z}+\tfrac{1}{2}.$$

It is seen that the second and fourth coordinates are obtained from the first and third coordinates, respectively, upon the addition of the vector $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. An additional I-centring is therefore present in this set of special positions. Hence, the special reflection condition for this set is hkl: $h + k + l = 2n$.

It should be pointed out, however, that only the general reflection conditions are used for a complete or partial determination of the space group and that the special reflection conditions only apply to spherical atoms. By the latter assumption we understand not only the assumption of spherical distribution of the atomic electron density but also isotropic displacement parameters of the equivalent atoms that belong to the set of corresponding special positions.

One method of finding the minimal special reflection conditions for a given set of special positions is the evaluation of the trigonometric structure factor for the set in question. For example, consider the Wyckoff position $4c$ of the space group $Pbcm$ (57). The coordinates of the special equivalent positions are

$$4c:\ x, \tfrac{1}{4}, 0;\quad \bar{x}, \tfrac{3}{4}, \tfrac{1}{2};\quad \bar{x}, \tfrac{3}{4}, 0;\quad x, \tfrac{1}{4}, \tfrac{1}{2}$$

and the corresponding trigonometric structure factor is

$$S(\mathbf{h}) = \exp\left[2\pi i\left(hx + \frac{k}{4}\right)\right] + \exp\left[2\pi i\left(-hx + \frac{3k}{4} + \frac{l}{2}\right)\right] + \exp\left[2\pi i\left(-hx + \frac{3k}{4}\right)\right] + \exp\left[2\pi i\left(hx + \frac{k}{4} + \frac{l}{2}\right)\right].$$

It can be easily shown that

$$S(\mathbf{h}) = 2\cos\left[2\pi\left(hx + \frac{k}{4}\right)\right][1 + \exp(\pi i l)]$$

and the last factor equals 2 for l even and equals zero for l odd. The special reflection condition is therefore: hkl: $l = 2n$.

Another approach is provided by considerations of the eigensymmetry group and the extraordinary orbits of the space group (see Section 1.4.4.4). We recall that the eigensymmetry group is a group of all the operations that leave the orbit of a point under the space group considered invariant, and the extraordinary orbit is associated with the eigensymmetry group that contains translations not present in the space group (see Chapter 1.4). In the above example the orbit is extraordinary, since its eigensymmetry group contains a translation corresponding to $\frac{1}{2}\mathbf{c}$. If this is taken as a basis vector, we have the Laue equation $\frac{1}{2}\mathbf{c}\cdot\mathbf{h} = l'$, where $\mathbf{h}$ is represented as a reciprocal-lattice vector and l' is an integer which also equals $l/2$. But for $l/2$ to be an integer we must have even l. We again obtain the condition hkl: $l = 2n$.

  references