Table 1.11.2.2. *The indices of the forbidden reflections and corresponding tensors of structure factors $F_{jk}(hk\ell)$ for the cubic space groups* ($n = 0, \pm1, \pm2, \ldots$)

Space group	Indices of reflections	Expressions for $F_{jk}(hk\ell)$ and additional restrictions
$P2_13$	00ℓ: $\ell = 2n+1$	(1.11.2.23)
$Pn\bar{3}$	$0k\ell$: $\ell = 2n+1$	(1.11.2.6); $F_2 = 0$ for 00ℓ
$Fd\bar{3}$	$0k\ell$: $k, \ell = 2n, k+\ell = 4n+2$	(1.11.2.6); $F_2 = 0$ for 00ℓ
$Pa\bar{3}$	$0k\ell$: $k = 2n+1$	(1.11.2.6); $F_2 = 0$ for $0k0$
$Ia\bar{3}$	$0k\ell$: $k, \ell = 2n+1$	(1.11.2.6)
$P4_232$	00ℓ: $\ell = 2n+1$	(1.11.2.24)
$F4_132$	00ℓ: $\ell = 4n+2$	(1.11.2.24)
$P4_332$	00ℓ: $\ell = 4n\pm1$	(1.11.2.23); $F_2 = \mp iF_1$
	00ℓ: $\ell = 4n+2$	(1.11.2.24)
$P1_332$	00ℓ: $\ell = 4n\pm1$	(1.11.2.23); $F_2 = \pm iF_1$
	00ℓ: $\ell = 4n+2$	(1.11.2.24)
$I4_132$	00ℓ: $\ell = 4n+2$	(1.11.2.24)
$P\bar{4}3n$	$hh\ell$: $\ell = 2n+1$	(1.11.2.22); $F_2 = 0$ for 00ℓ, $F_1 = F_2 = 0$ for hhh
$F\bar{4}3c$	$hh\ell$: $h, \ell = 2n+1$	(1.11.2.22); $F_1 = F_2 = 0$ for hhh
$I\bar{4}3d$	$hh\ell$: $2h+\ell = 4n+2$	(1.11.2.22); $F_2 = 0$ for 00ℓ, $F_1 = F_2 = 0$ for hhh
$Pn\bar{3}n$	$hh\ell$: $\ell = 2n+1$	(1.11.2.22); $F_1 = F_2 = 0$ for hhh
	$0k\ell$: $k+\ell = 2n+1$	(1.11.2.6); $F_1 = F_2 = 0$ for 00ℓ
$Pm\bar{3}n$	$hh\ell$: $\ell = 2n+1$	(1.11.2.22); $F_1 = F_2 = 0$ for hhh
$Pn\bar{3}m$	$0k\ell$: $k+\ell = 2n+1$	(1.11.2.6); $F_2 = 0$ for 00ℓ
$Fm\bar{3}c$	$hh\ell$: $h, \ell = 2n+1$	(1.11.2.22); $F_1 = F_2 = 0$ for hhh
$Fd\bar{3}m$	$0k\ell$: $k, \ell = 2n, k+\ell = 4n+2$	(1.11.2.6); $F_2 = 0$ for 00ℓ
$Fd\bar{3}c$	$0k\ell$: $k, \ell = 2n, k+\ell = 4n+2$	(1.11.2.6); $F_2 = 0$ for 00ℓ
	$hh\ell$: $h, \ell = 2n+1$	(1.11.2.22); $F_1 = F_2 = 0$ for hhh
$Ia\bar{3}d$	$0k\ell$: $k, \ell = 2n+1$	(1.11.2.6); $F_2 = -F_1$ for $0kk$
	$hh\ell$: $4h+\ell = 4n+2$	(1.11.2.22); hhh: $F_1 = F_2 = 0$, $F_2 = 0$ for 00ℓ

$Pn\bar{3}$: (1.11.2.10) and

$$a_i(x, y, z) = a_i(\tfrac{1}{2} - x, \tfrac{1}{2} - y, \tfrac{1}{2} - z). \qquad (1.11.2.13)$$

$Fd\bar{3}$: (1.11.2.10) and

$$a_i(x, y, z) = a_i(\tfrac{1}{4} - x, \tfrac{1}{4} - y, \tfrac{1}{4} - z). \qquad (1.11.2.14)$$

$Pa\bar{3}$, $Ia\bar{3}$: (1.11.2.11) and (1.11.2.12).
$P432$, $F432$, $I432$: (1.11.2.10) and

$$a_i(x, y, z) = a_i(\bar{x}, \bar{z}, \bar{y}). \qquad (1.11.2.15)$$

$P4_232$: (1.11.2.10) and

$$a_i(x, y, z) = a_i(\tfrac{1}{2} - x, \tfrac{1}{2} - z, \tfrac{1}{2} - y). \qquad (1.11.2.16)$$

$F4_132$, $P4_332$, $I4_132$: (1.11.2.11) and

$$a_i(x, y, z) = a_i(\tfrac{1}{4} - x, \tfrac{1}{4} - z, \tfrac{1}{4} - y). \qquad (1.11.2.17)$$

$P4_132$: (1.11.2.11) and

$$a_i(x, y, z) = a_i(\tfrac{3}{4} - x, \tfrac{3}{4} - z, \tfrac{3}{4} - y). \qquad (1.11.2.18)$$

$P\bar{4}3m$, $F\bar{4}3m$, $I\bar{4}3m$: (1.11.2.10) and

$$a_i(x, y, z) = a_i(x, z, y). \qquad (1.11.2.19)$$

$P\bar{4}3n$, $F\bar{4}3c$: (1.11.2.10) and

$$a_i(x, y, z) = a_i(\tfrac{1}{2} + x, \tfrac{1}{2} + z, \tfrac{1}{2} + y). \qquad (1.11.2.20)$$

$I\bar{4}3d$: (1.11.2.11) and

$$a_i(x, y, z) = a_i(\tfrac{1}{4} + x, \tfrac{1}{4} + z, \tfrac{1}{4} + y). \qquad (1.11.2.21)$$

$Pm\bar{3}m$, $Fm\bar{3}m$, $Im\bar{3}m$: (1.11.2.10), (1.11.2.12) and (1.11.2.19).
$Pn\bar{3}n$: (1.11.2.10), (1.11.2.13) and (1.11.2.15).
$Pm\bar{3}n$, $Fm\bar{3}c$: (1.11.2.10), (1.11.2.12) and (1.11.2.20).
$Pn\bar{3}m$: (1.11.2.10), (1.11.2.13) and (1.11.2.19).
$Fd\bar{3}m$: (1.11.2.10), (1.11.2.14) and (1.11.2.19).
$Fd\bar{3}c$: (1.11.2.10), (1.11.2.13) and (1.11.2.20).
$Ia\bar{3}d$: (1.11.2.11), (1.11.2.12) and (1.11.2.21).

For all $a_i(x, y, z)$, the sets of coordinates are chosen here as in *International Tables for Crystallography* Volume A (Hahn, 2005); the first one being adopted if Volume A offers two alternative origins. The expressions (1.11.2.10) or (1.11.2.11) appear for all space groups because all of them are supergroups of $P23$ or $P2_13$.

The tensor structure factors of forbidden reflections can be further restricted by the cubic symmetry, see Table 1.11.2.2. For the glide plane c, the tensor structure factor of $0k\ell$; $\ell = 2n+1$ reflections is given by (1.11.2.6), whereas for the diagonal glide plane n, it is given by

$$F_{jk}(hh\ell;\, \ell = 2n+1) = \begin{pmatrix} F_1 & 0 & F_2 \\ 0 & -F_1 & -F_2 \\ F_2 & -F_2 & 0 \end{pmatrix}, \qquad (1.11.2.22)$$

and additional restrictions on F_1 and F_2 can become effective for $k = \ell$ or $h = \ell$. For forbidden reflections of the 00ℓ type, the tensor structure factor is either

$$F_{jk}(00\ell) = \begin{pmatrix} 0 & 0 & F_1 \\ 0 & 0 & F_2 \\ F_1 & F_2 & 0 \end{pmatrix} \qquad (1.11.2.23)$$

or

$$F_{jk}(00\ell) = \begin{pmatrix} F_1 & F_2 & 0 \\ F_2 & -F_1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad (1.11.2.24)$$

see Table 1.11.2.2.

1.11.3. Polarization properties and azimuthal dependence

There are two important properties that distinguish forbidden reflections from conventional ('allowed') ones: non-trivial polarization effects and strong azimuthal dependence of intensity (and sometimes also of polarization) corresponding to the symmetry of the direction of the scattering vector. The azimuthal dependence means that the intensity and polarization properties of the reflection can change when the crystal is rotated around the direction of the reciprocal-lattice vector, *i.e.* they change with the azimuthal angle of the incident wavevector **k** defined relative to the scattering vector. The polarization and azimuthal properties, both mainly determined by symmetry, are two of the most informative characteristics of forbidden reflections. A third one, energy dependence, is determined by physical interactions, electronic and/or magnetic, where the role of symmetry is indirect but nevertheless also important (*e.g.* in splitting of atomic levels *etc.*, see Section 1.11.4).

In the kinematical theory, usually used for weak reflections, one obtains for unpolarized incident radiation the intensity of a conventional reflection as given by

$$I_{\mathbf{H}} = A_{\mathbf{H}} |F(\mathbf{H})|^2 \left(1 + \cos^2 2\theta\right)/2, \qquad (1.11.3.1)$$

where θ is the Bragg angle, $F(\mathbf{H})$ is the scalar structure factor of reflection **H**, and $A_{\mathbf{H}}$ is a scale factor, which depends on the incident beam intensity, the sample volume, the geometry of diffraction *etc.* (see *International Tables for Crystallography* Volume B), and can be set to $A_{\mathbf{H}} = 1$ hereafter.