International Tables for Crystallography (2010). Vol. B, Table 2.2.3.4, pp. 220–221.

Table 2.2.3.3. *Allowed origin translations, seminvariant moduli and phases for centrosymmetric non-primitive space groups*

	H–K group				
	$(h, l)\underline{C}(2, 2)$	$(k, l)\underline{I}(2, 2)$	$(h+k+l)\underline{F}(2)$	$(l)\underline{I}(2)$	$\underline{I}$
Space groups	$C\frac{2}{m}$	$Immm$	$Fmmm$	$I\frac{4}{m}$	$Im\bar{3}$
	$C\frac{2}{c}$	$Ibam$	$Fddd$	$I\frac{4_1}{a}$	$Ia\bar{3}$
	$Cmcm$	$Ibca$	$Fm\bar{3}$	$I\frac{4}{m}mm$	$Im\bar{3}m$
	$Cmca$	$Imma$	$Fd\bar{3}$	$I\frac{4}{m}cm$	$Ia\bar{3}d$
	$Cmmm$		$Fm\bar{3}m$	$I\frac{4_1}{a}md$	
	$Cccm$		$Fm\bar{3}c$	$I\frac{4_1}{a}cd$	
	$Cmma$		$Fd\bar{3}m$		
	$Ccca$		$Fd\bar{3}c$		
Allowed origin translations	(0, 0, 0) $(0, 0, \frac{1}{2})$ $(\frac{1}{2}, 0, 0)$ $(\frac{1}{2}, 0, \frac{1}{2})$	(0, 0, 0) $(0, 0, \frac{1}{2})$ $(0, \frac{1}{2}, 0)$ $(\frac{1}{2}, 0, 0)$	(0, 0, 0) $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(0, 0, 0) $(0, 0, \frac{1}{2})$	(0, 0, 0)
Vector $\mathbf{h}_s$ seminvariantly associated with $\mathbf{h} = (h, k, l)$	(h, l)	(k, l)	$(h+k+l)$	(l)	(h, k, l)
Seminvariant modulus $\boldsymbol{\omega}_s$	(2, 2)	(2, 2)	(2)	(2)	(1, 1, 1)
Seminvariant phases	φ_{eee}	φ_{eee}	φ_{eee}	φ_{eoe}; φ_{eee} φ_{ooe}; φ_{oee}	All
Number of semindependent phases to be specified	2	2	1	1	0

(2) treatment of missing weak data (Rogers *et al.*, 1955; Vicković & Viterbo, 1979). All unobserved reflections may assume

$$\mu = |F_{\rm o\,min}|^2/3 \text{ for cs. space groups}$$
$$\mu = |F_{\rm o\,min}|^2/2 \text{ for ncs. space groups,}$$

where the subscript 'o min' refers to the minimum observed intensity.

Once K and B have been estimated, $E_{\mathbf{h}}$ values can be obtained from experimental data by

$$|E_{\mathbf{h}}|^2 = \frac{KI_{\mathbf{h}}}{\langle |F^{\rm o}_{\mathbf{h}}|^2\rangle \exp(-2Bs^2)},$$

Table 2.2.3.4. *Allowed origin translations, seminvariant moduli and phases for noncentrosymmetric non-primitive space groups*

	H–K group					
	$(k, l)C(0, 2)$	$(h, l)C(0, 0)$	$(h, l)C(2, 0)$	$(h, l)C(2, 2)$	$(h, l)A(2, 0)$	$(h, l)I(2, 0)$
Space group	$C2$	Cm Cc	$Cmm2$ $Cmc2_1$ $Ccc2$	$C222$ $C222_1$	$Amm2$ $Abm2$ $Ama2$ $Aba2$	$Imm2$ $Iba2$ $Ima2$
Allowed origin translations	$(0, y, 0)$ $(0, y, \frac{1}{2})$	$(x, 0, z)$	$(0, 0, z)$ $(\frac{1}{2}, 0, z)$	(0, 0, 0) $(0, 0, \frac{1}{2})$ $(\frac{1}{2}, 0, 0)$ $(\frac{1}{2}, 0, \frac{1}{2})$	$(0, 0, z)$ $(\frac{1}{2}, 0, z)$	$(0, 0, z)$ $(\frac{1}{2}, 0, z)$
Vector $\mathbf{h}_s$ seminvariantly associated with $\mathbf{h} = (h, k, l)$	(k, l)	(h, l)	(h, l)	(h, l)	(h, l)	(h, l)
Seminvariant modulus $\boldsymbol{\omega}_s$	(0, 2)	(0, 0)	(2, 0)	(2, 2)	(2, 0)	(2, 0)
Seminvariant phases	φ_{e0e}	φ_{0e0}	φ_{ee0}	φ_{eee}	φ_{ee0}	φ_{ee0}
Allowed variations for the semindependent phases	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $k = 0$	$\Vert\infty\Vert$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $l = 0$	$\Vert 2\Vert$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $l = 0$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $l = 0$
Number of semindependent phases to be specified	2	2	2	2	2	2

where $\langle |F_{\mathbf{h}}^{\rm o}|^2 \rangle$ is the expected value of $|F_{\mathbf{h}}^{\rm o}|^2$ for the reflection $\mathbf{h}$ on the basis of the available *a priori* information.

2.2.4.4. Probability distributions of normalized structure factors

Under some fairly general assumptions (see Chapter 2.1) probability distribution functions for the variable $|E|$ for cs. and ncs. structures are (see Fig. 2.2.4.1)

$$ {}_{\bar{1}}P(|E|)\,{\rm d}|E| = \sqrt{\frac{2}{\pi}}\exp\left(-\frac{E^2}{2}\right){\rm d}|E| \qquad (2.2.4.4)$$

and

$$ {}_{1}P(|E|)\,{\rm d}|E| = 2|E|\exp(-|E|^2)\,{\rm d}|E|, \qquad (2.2.4.5)$$

respectively. Corresponding cumulative functions are (see Fig. 2.2.4.2)

$$ {}_{\bar{1}}N(|E|) = \sqrt{\frac{2}{\pi}}\int\limits_0^{|E|}\exp\left(-\frac{t^2}{2}\right){\rm d}t = {\rm erf}\left(\frac{|E|}{\sqrt{2}}\right),$$

$$ {}_{1}N(|E|) = \int\limits_0^{|E|} 2t\exp(-t^2)\,{\rm d}t = 1-\exp(-|E|^2).$$

Some moments of the distributions (2.2.4.4) and (2.2.4.5) are listed in Table 2.2.4.1. In the absence of other indications for a given crystal structure, a cs. or an ncs. space group will be preferred according to whether the statistical tests yield values closer to column 2 or to column 3 of Table 2.2.4.1.

For further details about the distribution of intensities see Chapter 2.1.

2.2.5. Phase-determining formulae

From the earliest periods of X-ray structure analysis several authors (Ott, 1927; Banerjee, 1933; Avrami, 1938) have tried to determine atomic positions directly from diffraction intensities.

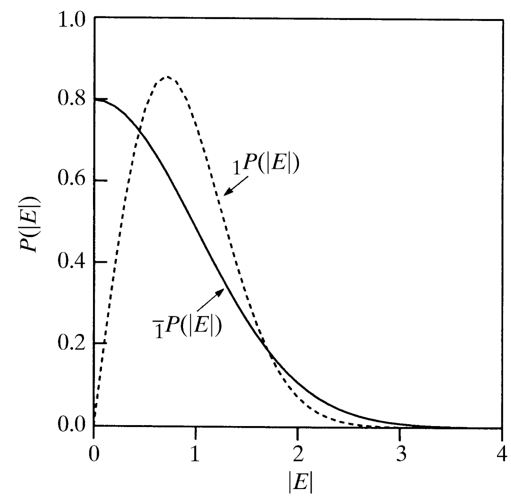

Fig. 2.2.4.1. Probability density functions for cs. and ncs. crystals.

Significant developments are the derivation of inequalities and the introduction of probabilistic techniques *via* the use of joint probability distribution methods (Hauptman & Karle, 1953).

2.2.5.1. Inequalities among structure factors

An extensive system of inequalities exists for the coefficients of a Fourier series which represents a positive function. This can restrict the allowed values for the phases of the s.f.'s in terms of measured structure-factor magnitudes. Harker & Kasper (1948) derived two types of inequalities:

Type 1. A modulus is bound by a combination of structure factors:

$$|U_{\mathbf{h}}|^2 \le \frac{1}{m}\sum_{s=1}^{m} a_s(-\mathbf{h})U_{\mathbf{h}(\mathbf{I}-\mathbf{R}_s)}, \qquad (2.2.5.1)$$

where m is the order of the point group and $a_s(-\mathbf{h}) = \exp(-2\pi i\mathbf{h}\cdot\mathbf{T}_s)$.

Table 2.2.3.4 (*cont.*)

$(h, l)I(2, 2)$	$(h+k+l)F(2)$	$(h+k+l)F(4)$	$(l)I(0)$	$(l)I(2)$	$(2k-l)I(4)$	$(l)F(0)$	I
$I222$ $I2_12_12_1$	$F432$ $F4_132$	$F222$ $F23$ $F\bar{4}3m$ $F\bar{4}3c$	$I4$ $I4_1$ $I4mm$ $I4cm$ $I4_1md$ $I4_1cd$	$I422$ $I4_122$ $I\bar{4}2m$ $I\bar{4}2d$	$I\bar{4}$ $I\bar{4}m2$ $I\bar{4}c2$	$Fmm2$ $Fdd2$	$I23$ $I2_13$ $I432$ $I4_132$ $I\bar{4}3m$ $I\bar{4}3d$
(0, 0, 0) $(0, 0, \frac{1}{2})$ $(0, \frac{1}{2}, 0)$ $(\frac{1}{2}, 0, 0)$	(0, 0, 0) $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	(0, 0, 0) $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$	$(0, 0, z)$	(0, 0, 0) $(0, 0, \frac{1}{2})$	(0, 0, 0) $(0, 0, \frac{1}{2})$ $(\frac{1}{2}, 0, \frac{3}{4})$ $(\frac{1}{2}, 0, \frac{1}{4})$	$(0, 0, z)$	(0, 0, 0)
(h, l)	$(h+k+l)$	$(h+k+l)$	(l)	(l)	$(2k-l)$	(l)	(h, k, l)
(2, 2)	(2)	(4)	(0)	(2)	(4)	(0)	(1, 1, 1)
$\varphi_{\rm eee}$	$\varphi_{\rm eee}$	φ_{hkl} with $h+k+l\equiv 0$ (mod 4)	φ_{hk0}	φ_{hke}	φ_{hkl} with $(2k-l)\equiv 0$ (mod 4)	φ_{hk0}	All
$\|2\|$	$\|2\|$	$\|2\|$ if $h+k+l\equiv 0$ (mod 2) $\|4\|$ if $h+k+l\equiv 1$ (mod 2)	$\|\infty\|$	$\|2\|$	$\|2\|$ if $h+k+l\equiv 0$ (mod 2) $\|4\|$ if $2k-l\equiv 1$ (mod 2)	$\|\infty\|$	All
2	1	1	1	1	1	1	0