

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

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

	H-K group				
	$(h, l)C(2, 2)$	$(k, l)I(2, 2)$	$(h + k + l)F(2)$	$(l)I(2)$	I
Space groups	$C\frac{2}{m}$ $C\frac{2}{c}$ <i>Cmcm</i> <i>Cmca</i> <i>Cmmm</i> <i>Cccm</i> <i>Cmma</i> <i>Ccca</i>	<i>Immm</i> <i>Ibam</i> <i>Ibca</i> <i>Imma</i>	<i>Fmmm</i> <i>Fddd</i> <i>Fm$\bar{3}$</i> <i>Fd$\bar{3}$</i> <i>Fm$\bar{3}m$</i> <i>Fm$\bar{3}c$</i> <i>Fd$\bar{3}m$</i> <i>Fd$\bar{3}c$</i>	$I\frac{4}{m}$ $I\frac{4}{a}$ $I\frac{4}{m}mm$ $I\frac{4}{m}cm$ $I\frac{4}{a}md$ $I\frac{4}{a}cd$	<i>Im$\bar{3}$</i> <i>Ia$\bar{3}$</i> <i>Im$\bar{3}m$</i> <i>Ia$\bar{3}d$</i>
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 ω_s	(2, 2)	(2, 2)	(2)	(2)	(1, 1, 1)
Seminvariant phases	φ_{eee}	φ_{eee}	φ_{eee}	$\varphi_{eoe}; \varphi_{eee}$ $\varphi_{oee}; \varphi_{oee}$	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

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

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

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

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

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	<i>C2</i>	<i>Cm</i> <i>Cc</i>	<i>Cmm2</i> <i>Cmc2₁</i> <i>Ccc2</i>	<i>C222</i> <i>C222₁</i>	<i>Amm2</i> <i>Abm2</i> <i>Ama2</i> <i>Aba2</i>	<i>Imm2</i> <i>Iba2</i> <i>Ima2</i>
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 ω_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	$\ \infty\ , \ 2\ $ if $k = 0$	$\ \infty\ $	$\ \infty\ , \ 2\ $ if $l = 0$	$\ 2\ $	$\ \infty\ , \ 2\ $ if $l = 0$	$\ \infty\ , \ 2\ $ if $l = 0$
Number of semindependent phases to be specified	2	2	2	2	2	2