Table 2.2.3.1. *Allowed origin translations, seminvariant moduli and phases for centrosymmetric primitive space groups*

	H–K group					
	$(h, k, l)\underline{P}(2, 2, 2)$		$(h+k, l)\underline{P}(2, 2)$		$(l)\underline{P}(2)$	$(h+k+l)\underline{P}(2)$
Space group	$P\bar{1}$	$Pmna$	$P\frac{4}{m}$	$P\frac{4}{n}mm$	$P\bar{3}$	$R\bar{3}$
	$P\frac{2}{m}$	$Pcca$	$P\frac{4_2}{m}$	$P\frac{4}{n}cc$	$P\bar{3}1m$	$R\bar{3}m$
	$P\frac{2_1}{m}$	$Pbam$	$P\frac{4}{n}$	$P\frac{4_2}{m}mc$	$P\bar{3}1c$	$R\bar{3}c$
	$P\frac{2}{c}$	$Pccn$	$P\frac{4_2}{n}$	$P\frac{4_2}{m}cm$	$P\bar{3}m1$	$Pm\bar{3}$
	$P\frac{2_1}{c}$	$Pbcm$	$P\frac{4}{m}mm$	$P\frac{4_2}{n}bc$	$P\bar{3}c1$	$Pn\bar{3}$
	$Pmmm$	$Pnnm$	$P\frac{4}{m}cc$	$P\frac{4_2}{n}nm$	$P\frac{6}{m}$	$Pa\bar{3}$
	$Pnnn$	$Pmmn$	$P\frac{4}{n}bm$	$P\frac{4_2}{m}bc$	$P\frac{6_3}{m}$	$Pm\bar{3}m$
	$Pccm$	$Pbcn$	$P\frac{4}{n}nc$	$P\frac{4_2}{m}nm$	$P\frac{6}{m}mm$	$Pn\bar{3}n$
	$Pban$	$Pbca$	$P\frac{4}{m}bm$	$P\frac{4_2}{n}mc$	$P\frac{6}{m}cc$	$Pm\bar{3}n$
	$Pmma$	$Pnma$	$P\frac{4}{m}nc$	$P\frac{4_2}{n}cm$	$P\frac{6_3}{m}cm$	$Pn\bar{3}m$
	$Pnna$				$P\frac{6_3}{m}mc$	
Allowed origin translations	$(0, 0, 0)$; $(\frac{1}{2}, 0, 0)$; $(0, \frac{1}{2}, 0)$; $(0, 0, \frac{1}{2})$;	$(0, \frac{1}{2}, \frac{1}{2})$ $(\frac{1}{2}, 0, \frac{1}{2})$ $(\frac{1}{2}, \frac{1}{2}, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(0, 0, 0)$ $(0, 0, \frac{1}{2})$ $(\frac{1}{2}, \frac{1}{2}, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		$(0, 0, 0)$ $(0, 0, \frac{1}{2})$	$(0, 0, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
Vector $\mathbf{h}_s$ seminvariantly associated with $\mathbf{h} = (h, k, l)$	(h, k, l)		$(h+k, l)$		(l)	$(h+k+l)$
Seminvariant modulus $\boldsymbol{\omega}_s$	(2, 2, 2)		(2, 2)		(2)	(2)
Seminvariant phases	φ_{eee}		φ_{eee}; φ_{ooe}		φ_{eee}; φ_{eoe} φ_{oee}; φ_{ooe}	φ_{eee}; φ_{ooe} φ_{oeo}; φ_{eoo}
Number of semindependent phases to be specified	3		2		1	1

where $|F_{\mathbf{h}}|^2$ is the squared observed structure-factor magnitude on the absolute scale and $\langle|F_{\mathbf{h}}|^2\rangle$ is the expected value of $|F_{\mathbf{h}}|^2$.

$\langle|F_{\mathbf{h}}|^2\rangle$ depends on the available *a priori* information. Often, but not always, this may be considered as a combination of several typical situations. We mention:

(*a*) No structural information. The atomic positions are considered random variables. Then

$$\langle|F_{\mathbf{h}}|^2\rangle = \varepsilon_{\mathbf{h}} \sum_{j=1}^{N} f_j^2 = \varepsilon_{\mathbf{h}} \sum\nolimits_N$$

so that

$$E_{\mathbf{h}} = \frac{F_{\mathbf{h}}}{(\varepsilon_{\mathbf{h}} \sum\nolimits_N)^{1/2}}. \qquad (2.2.4.2)$$

$\varepsilon_{\mathbf{h}}$ takes account of the effect of space-group symmetry (see Chapter 2.1).

(*b*) P atomic groups having a known configuration but with unknown orientation and position (Main, 1976). Then a certain number of interatomic distances $r_{j_1 j_2}$ are known and

$$\langle|F_{\mathbf{h}}|^2\rangle = \varepsilon_{\mathbf{h}} \left(\sum\nolimits_N + \sum_{i=1}^{P} \sum_{j_1 \neq j_2 = 1}^{M_i} f_{j_1} f_{j_2} \frac{\sin 2\pi q r_{j_1 j_2}}{2\pi q r_{j_1 j_2}} \right),$$

where M_i is the number of atoms in the ith molecular fragment and $q = |\mathbf{h}|$.

(*c*) P atomic groups with a known configuration, correctly oriented, but with unknown position (Main, 1976). Then a certain group of interatomic vectors $\mathbf{r}_{j_1 j_2}$ is fixed and

$$\langle|F_{\mathbf{h}}|^2\rangle = \varepsilon_{\mathbf{h}} \left(\sum\nolimits_N + \sum_{i=1}^{P} \sum_{j_1 \neq j_2 = 1}^{M_i} f_{j_1} f_{j_2} \exp 2\pi i \mathbf{h} \cdot \mathbf{r}_{j_1 j_2} \right).$$

The above formula has been derived on the assumption that primitive positional random variables are uniformly distributed over the unit cell. Such an assumption may be considered unfavourable (Giacovazzo, 1988) in space groups for which the allowed shifts of origin, consistent with the chosen algebraic form for the symmetry operators $\mathbf{C}_s$, are arbitrary displacements along any polar axes. Thanks to the indeterminacy in the choice of origin, the first of the shifts $\boldsymbol{\tau}_i$ (to be applied to the ith fragment in order to translate atoms in the correct positions) may be restricted to a region which is smaller than the unit cell (*e.g.* in $P2$ we are free to specify the origin along the diad axis by restricting $\boldsymbol{\tau}_1$ to the family of vectors $\{\boldsymbol{\tau}_1\}$ of type $[x0z]$). The practical consequence is that $\langle|F_{\mathbf{h}}|^2\rangle$ is significantly modified in polar space groups if $\mathbf{h}$ satisfies

$$\mathbf{h} \cdot \boldsymbol{\tau}_1 = 0,$$

where $\boldsymbol{\tau}_1$ belongs to the family of restricted vectors $\{\boldsymbol{\tau}_1\}$.

(*d*) Atomic groups correctly positioned. Then (Main, 1976; Giacovazzo, 1983*a*)

references