International Tables for Crystallography (2010). Vol. B, Table 2.2.3.2, pp. 218–219.

$$\langle|F_{\mathbf{h}}|^2\rangle = |F_{\mathrm{p},\,\mathbf{h}}|^2 + \varepsilon_{\mathbf{h}} \textstyle\sum_q,$$

where $F_{\mathrm{p},\mathbf{h}}$ is the structure factor of the partial known structure and q are the atoms with unknown positions.

(*e*) A pseudotranslational symmetry is present. Let $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \ldots$ be the pseudotranslation vectors of order $n_1, n_2, n_3, \ldots$, respectively. Furthermore, let p be the number of atoms (symmetry equivalents included) whose positions are related by pseudotranslational symmetry and q the number of atoms (symmetry equivalents included) whose positions are not related by any pseudotranslation. Then (Cascarano *et al.*, 1985*a*,*b*)

$$\langle|F_{\mathbf{h}}|^2\rangle = \varepsilon_{\mathbf{h}}(\zeta_{\mathbf{h}} \textstyle\sum_p + \sum_q),$$

where

$$\zeta_{\mathbf{h}} = \frac{(n_1 n_2 n_3 \ldots)\gamma_{\mathbf{h}}}{m}$$

and $\gamma_{\mathbf{h}}$ is the number of times for which algebraic congruences

$$\mathbf{h} \cdot \mathbf{R}_s \mathbf{u}_i \equiv 0 \ (\mathrm{mod}\ 1) \quad \text{for } i = 1, 2, 3, \ldots$$

are simultaneously satisfied when s varies from 1 to m. If $\gamma_{\mathbf{h}} = 0$ then $F_{\mathbf{h}}$ is said to be a *superstructure reflection*, otherwise it is a *substructure reflection.*

Often substructures are not ideal: *e.g.* atoms related by pseudotranslational symmetry are ideally located but of different type (replacive deviations from ideality); or they are equal but not ideally located (displacive deviations); or a combination of the two situations occurs. In these cases a correlation exists between the substructure and the superstructure. It has been shown (Mackay, 1953; Cascarano *et al.*, 1988*a*) that the scattering power of the substructural part may be estimated *via* a statistical analysis of diffraction data for ideal pseudotranslational symmetry or for displacive deviations from it, while it is not estimable in the case of replacive deviations.

2.2.4.2. *Definition of quasi-normalized structure factor*

When probability theory is not used, the *quasi-normalized structure factors* $\mathcal{E}_{\mathbf{h}}$ and the *unitary structure factors* $U_{\mathbf{h}}$ are often used. $\mathcal{E}_{\mathbf{h}}$ and $U_{\mathbf{h}}$ are defined according to

$$|\mathcal{E}_{\mathbf{h}}|^2 = \varepsilon_{\mathbf{h}}|E_{\mathbf{h}}|^2$$

$$U_{\mathbf{h}} = F_{\mathbf{h}} \bigg/ \left(\sum_{j=1}^{N} f_j\right).$$

Since $\sum_{j=1}^{N} f_j$ is the largest possible value for $F_{\mathbf{h}}$, $U_{\mathbf{h}}$ represents the fraction of $F_{\mathbf{h}}$ with respect to its largest possible value. Therefore

Table 2.2.3.2. *Allowed origin translations, seminvariant moduli and phases for noncentrosymmetric primitive space groups*

	H–K group					
	$(h, k, l)P(0, 0, 0)$	$(h, k, l)P(2, 0, 2)$	$(h, k, l)P(0, 2, 0)$	$(h, k, l)P(2, 2, 2)$	$(h, k, l)P(2, 2, 0)$	$(h+k, l)P(2, 0)$
Space group	$P1$	$P2$ $P2_1$	Pm Pc	$P222$ $P222_1$ $P2_12_12$ $P2_12_12_1$	$Pmm2$ $Pmc2_1$ $Pcc2$ $Pma2$ $Pca2_1$ $Pnc2$ $Pmn2_1$ $Pba2$ $Pna2_1$ $Pnn2$	$P4$ $P4_1$ $P4_2$ $P4_3$ $P4mm$ $P4bm$ $P4_2cm$ $P4_2nm$ $P4cc$ $P4nc$ $P4_2mc$ $P4_2bc$
Allowed origin translations	(x, y, z)	$(0, y, 0)$ $(0, y, \frac{1}{2})$ $(\frac{1}{2}, y, 0)$ $(\frac{1}{2}, y, \frac{1}{2})$	$(x, 0, z)$ $(x, \frac{1}{2}, z)$	$(0, 0, 0)$ $(\frac{1}{2}, 0, 0)$ $(0, \frac{1}{2}, 0)$ $(0, 0, \frac{1}{2})$ $(0, \frac{1}{2}, \frac{1}{2})$ $(\frac{1}{2}, 0, \frac{1}{2})$ $(\frac{1}{2}, \frac{1}{2}, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(0, 0, z)$ $(0, \frac{1}{2}, z)$ $(\frac{1}{2}, 0, z)$ $(\frac{1}{2}, \frac{1}{2}, z)$	$(0, 0, z)$ $(\frac{1}{2}, \frac{1}{2}, z)$
Vector $\mathbf{h}_s$ seminvariantly associated with $\mathbf{h} = (h, k, l)$	(h, k, l)	(h, k, l)	(h, k, l)	(h, k, l)	(h, k, l)	$(h + k, l)$
Seminvariant modulus $\boldsymbol{\omega}_s$	$(0, 0, 0)$	$(2, 0, 2)$	$(0, 2, 0)$	$(2, 2, 2)$	$(2, 2, 0)$	$(2, 0)$
Seminvariant phases	φ_{000}	φ_{e0e}	φ_{0e0}	φ_{eee}	φ_{ee0}	φ_{ee0} φ_{oo0}
Allowed variations for the semindependent phases	$\Vert\infty\Vert$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $k = 0$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $h = l = 0$	$\Vert 2\Vert$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $l = 0$	$\Vert\infty\Vert$, $\Vert 2\Vert$ if $l = 0$
Number of semindependent phases to be specified	3	3	3	3	3	2

$$0 \le |U_{\mathbf{h}}| \le 1.$$

If atoms are equal, then $U_{\mathbf{h}} = \mathscr{E}_{\mathbf{h}}/N^{1/2}$.

2.2.4.3. The calculation of normalized structure factors

N.s.f.'s cannot be calculated by applying (2.2.4.1) to observed s.f.'s because: (*a*) the observed magnitudes $I_{\mathbf{h}}$ (already corrected for Lp factor, absorption, ...) are on a relative scale; (*b*) $\langle |F_{\mathbf{h}}|^2 \rangle$ cannot be calculated without having estimated the vibrational motion of the atoms.

This is usually obtained by the well known Wilson plot (Wilson, 1942), according to which observed data are divided into ranges of $s^2 = \sin^2\theta/\lambda^2$ and averages of intensity $\langle I_{\mathbf{h}} \rangle$ are taken in each shell. Reflection multiplicities and other effects of space-group symmetry on intensities must be taken into account when such averages are calculated. The shells are symmetrically overlapped in order to reduce statistical fluctuations and are restricted so that the number of reflections in each shell is reasonably large. For each shell

$$K\langle I \rangle = \langle |F|^2 \rangle = \langle |F^{\rm o}|^2 \rangle \exp(-2Bs^2) \qquad (2.2.4.3)$$

should be obtained, where K is the scale factor needed to place X-ray intensities on the absolute scale, B is the overall thermal parameter and $\langle |F^{\rm o}|^2 \rangle$ is the expected value of $|F|^2$ in which it is assumed that all the atoms are at rest. $\langle |F^{\rm o}|^2 \rangle$ depends upon the structural information that is available (see Section 2.2.4.1 for some examples).

Equation (2.2.4.3) may be rewritten as

$$\ln\left\{\frac{\langle I \rangle}{\langle |F^{\rm o}|^2 \rangle}\right\} = -\ln K - 2Bs^2,$$

which plotted at various s^2 should be a straight line of which the slope ($2B$) and intercept ($\ln K$) on the logarithmic axis can be obtained by applying a linear least-squares procedure.

Very often molecular geometries produce perceptible departures from linearity in the logarithmic Wilson plot. However, the more extensive the available *a priori* information on the structure is, the closer, on the average, are the Wilson-plot curves to their least-squares straight lines.

Accurate estimates of B and K require good strategies (Rogers & Wilson, 1953) for:

(1) treatment of weak measured data. If weak data are set to zero, there will be bias in the statistics. Methods are, however, available (French & Wilson, 1978) that provide an *a posteriori* estimate of weak (even negative) intensities by means of Bayesian statistics.

Table 2.2.3.2 (*cont.*)

$(h+k, l)P(2, 2)$	$(h-k, l)P(3, 0)$	$(2h+4k+3l)P(6)$	$(l)P(0)$	$(l)P(2)$	$(h+k+l)P(0)$	$(h+k+l)P(2)$
$P\bar{4}$ $P422$ $P42_12$ $P4_122$ $P4_12_12$ $P4_222$ $P4_22_12$ $P4_322$ $P4_32_12$ $P\bar{4}2m$ $P\bar{4}2c$ $P\bar{4}2_1m$ $P\bar{4}2_1c$ $P\bar{4}m2$ $P\bar{4}c2$ $P\bar{4}b2$ $P\bar{4}n2$	$P3$ $P3_1$ $P3_2$ $P3m1$ $P3c1$	$P312$ $P3_112$ $P3_212$ $P6$ $P\bar{6}m2$ $P\bar{6}c2$	$P31m$ $P31c$ $P6$ $P6_1$ $P6_5$ $P6_4$ $P6_3$ $P6_2$ $P6mm$ $P6cc$ $P6_3cm$ $P6_3mc$	$P321$ $P3_121$ $P3_221$ $P622$ $P6_122$ $P6_522$ $P6_222$ $P6_422$ $P6_322$ $P\bar{6}2m$ $P\bar{6}2c$	$R3$ $R3m$ $R3c$	$R32$ $P23$ $P2_13$ $P432$ $P4_232$ $P4_332$ $P4_132$ $P\bar{4}3m$ $P\bar{4}3n$
$(0, 0, 0)$ $(0, 0, \frac{1}{2})$ $(\frac{1}{2}, \frac{1}{2}, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(0, 0, z)$ $(\frac{1}{3}, \frac{2}{3}, z)$ $(\frac{2}{3}, \frac{1}{3}, z)$	$(0, 0, 0)$ $(0, 0, \frac{1}{2})$ $(\frac{1}{3}, \frac{2}{3}, 0)$ $(\frac{1}{3}, \frac{2}{3}, \frac{1}{2})$ $(\frac{2}{3}, \frac{1}{3}, 0)$ $(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$	$(0, 0, z)$	$(0, 0, 0)$ $(0, 0, \frac{1}{2})$	(x, x, x)	$(0, 0, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
$(h+k, l)$	$(h-k, l)$	$(2h+4k+3l)$	(l)	(l)	$(h+k+l)$	$(h+k+l)$
$(2, 2)$	$(3, 0)$	(6)	(0)	(2)	(0)	(2)
$\varphi_{\rm eee}$ $\varphi_{\rm ooe}$	φ_{hk0} if $h-k=0$ (mod 3)	φ_{hkl} if $2h+4k+3l=0$ (mod 6)	φ_{hk0}	φ_{hke}	$\varphi_{h,k,\bar{h}+\bar{k}}$	$\varphi_{\rm eee}$; $\varphi_{\rm ooe}$ $\varphi_{\rm oeo}$; $\varphi_{\rm ooe}$
$\|2\|$	$\|\infty\|$, $\|3\|$ if $l=0$	$\|2\|$ if $h \equiv k$ (mod 3) $\|3\|$ if $l \equiv 0$ (mod 2)	$\|\infty\|$	$\|2\|$	$\|\infty\|$	$\|2\|$
2	2	1	1	1	1	1

references