(*a*) *No structural information*
(2.2.5.14) then reduces to (2.2.5.6).

(*b*) *Randomly positioned and randomly oriented atomic groups*
Then

$$g_i(\mathbf{h}_1,\mathbf{h}_2,\mathbf{h}_3) = \sum_{j,k,l} f_j f_k f_l \langle \exp[2\pi i(\mathbf{h}_1\cdot\mathbf{r}_{kj} + \mathbf{h}_2\cdot\mathbf{r}_{lj})]\rangle_R,$$

where $\langle\ldots\rangle_R$ means rotational average. The average of the exponential term extends over all orientations of the triangle formed by the atoms j, k and l, and is given (Hauptman, 1965) by

$$\begin{aligned} B(z,t) &= \langle \exp[2\pi i(\mathbf{h}\cdot\mathbf{r} + \mathbf{h}'\cdot\mathbf{r}')]\rangle \\ &= \left(\frac{\pi}{2z}\right)^{1/2} \sum_{n=0}^{\infty} \frac{t^{2n}}{(n!)^2} J_{(4n+1)/2}(z), \end{aligned}$$

where

$$z = 2\pi[q^2r^2 + 2qrq'r'\cos\varphi_q\cos\varphi_r + q'^2r'^2]^{1/2}$$

and

$$t = [2\pi^2 qrq'r'\sin\varphi_q\sin\varphi_r]/z;$$

q, q', r and r' are the magnitudes of $\mathbf{h}$, $\mathbf{h}'$, $\mathbf{r}$ and $\mathbf{r}'$, respectively; φ_q and φ_r are the angles $(\mathbf{h},\mathbf{h}')$ and $(\mathbf{r},\mathbf{r}')$, respectively.

(*c*) *Randomly positioned but correctly oriented atomic groups*
Then

$$\begin{aligned} g_i(\mathbf{h}_1,\mathbf{h}_2,\mathbf{h}_3) = \sum_{s=1}^{m} \sum_{j,k,l} & f_j f_k f_l \\ & \times \exp[2\pi i(\mathbf{h}_1\cdot\mathbf{R}_s\mathbf{r}_{kj} + \mathbf{h}_2\cdot\mathbf{R}_s\mathbf{r}_{lk})], \end{aligned}$$

where the summations over j, k, l are taken over all the atoms in the ith group.

A modified expression for g_i has to be used in polar space groups for special triplets (Giacovazzo, 1988).

Translation functions [see Chapter 2.3; for an overview, see also Beurskens *et al.* (1987)] are also used to determine the position of a correctly oriented molecular fragment.

Such functions can work in direct space [expressed as Patterson convolutions (Buerger, 1959; Nordman, 1985) or electron-density convolutions (Rossmann *et al.*, 1964; Argos & Rossmann, 1980)] or in reciprocal space [expressed as correlation functions (Crowther & Blow, 1967; Karle, 1972; Langs, 1985) or residual functions (Rae, 1977)]. Both the probabilistic methods and the translation functions are quite efficient tools: the decision as to which one to use is often a personal choice.

(*d*) *Atomic groups correctly positioned*
Let p be the number of atoms with known position, q the number of atoms with unknown position, F_p and F_q the corresponding structure factors.

Tangent recycling methods (Karle, 1970*b*) may be used for recovering the complete crystal structure. The phase $\varphi_{p,\mathbf{h}}$ is accepted in the starting set as a useful approximation of $\varphi_{\mathbf{h}}$ if $|F_{p,\mathbf{h}}| > \eta|F_{\mathbf{h}}|$, where η is the fraction of the total scattering power contained in the fragment and where $|F_{\mathbf{h}}|$ is associated with $|E_{\mathbf{h}}| > 1.5$.

Tangent recycling methods are applied (Beurskens *et al.*, 1979) with greater effectiveness to difference s.f.'s $\Delta F = (|F| - |F_p|)\exp(i\varphi_p)$. The weighted tangent formula uses $\Delta F_{\mathbf{h}}$ values in order to convert them to more probable $F_{q,\mathbf{h}}$ values.

From a probabilistic point of view (Giacovazzo, 1983*a*; Camalli *et al.*, 1985) the distribution of $\varphi_{\mathbf{h}}$, given $E'_{p,\mathbf{h}}$ and some products $(E'_{\mathbf{k}} - E'_{p,\mathbf{k}})(E'_{\mathbf{h}-\mathbf{k}} - E'_{p,\mathbf{h}-\mathbf{k}})$, is the von Mises function

$$P(\varphi_{\mathbf{h}}|\ldots) = [2\pi I_0(\alpha)]^{-1}\exp[\alpha\cos(\varphi_{\mathbf{h}} - \theta_{\mathbf{h}})], \qquad (2.2.5.15)$$

where $\theta_{\mathbf{h}}$, the most probable value of $\varphi_{\mathbf{h}}$, is given by

$$\begin{aligned} \tan\theta_{\mathbf{h}} &\simeq \alpha'_2/\alpha'_1, \qquad (2.2.5.16) \\ \alpha^2 &= \alpha'^2_1 + \alpha'^2_2 \end{aligned}$$

and

$$\begin{aligned} \alpha'_1 = 2R'_{\mathbf{h}}\Big\{\mathscr{R}\Big[E'_{p,\mathbf{h}} + q^{-1/2}\textstyle\sum_{\mathbf{k}}(E'_{\mathbf{k}} - E'_{p,\mathbf{k}}) \\ \times (E'_{\mathbf{h}-\mathbf{k}} - E'_{p,\mathbf{h}-\mathbf{k}})\Big]\Big\} \\ \alpha'_2 = 2R'_{\mathbf{h}}\Big\{\mathscr{I}\Big[E'_{p,\mathbf{h}} + q^{-1/2}\textstyle\sum_{\mathbf{k}}(E'_{\mathbf{k}} - E'_{p,\mathbf{k}}) \\ \times (E'_{\mathbf{h}-\mathbf{k}} - E'_{p,\mathbf{h}-\mathbf{k}})\Big]\Big\}. \end{aligned}$$

$\mathscr{R}$ and $\mathscr{I}$ stand for 'real and imaginary part of', respectively. Furthermore, $E' = F/\sum_q^{1/2}$ is a pseudo-normalized s.f. If no pair $(\varphi_{\mathbf{k}},\varphi_{\mathbf{h}-\mathbf{k}})$ is known, then

$$\begin{aligned} \alpha'_1 &= 2R'_{\mathbf{h}}R'_{p,\mathbf{h}}\cos\varphi_{p,\mathbf{h}} \\ \alpha'_2 &= 2R'_{\mathbf{h}}R'_{p,\mathbf{h}}\sin\varphi_{p,\mathbf{h}} \end{aligned}$$

and (2.2.5.15) reduces to Sim's (1959) equation

$$P(\varphi_{\mathbf{h}}) \simeq [2\pi I_0(G)]^{-1}\exp[G\cos(\varphi_{\mathbf{h}} - \varphi_{p,\mathbf{h}})], \qquad (2.2.5.17)$$

where $G = 2R'_{\mathbf{h}}R'_{p,\mathbf{h}}$. In this case $\varphi_{p,\mathbf{h}}$ is the most probable value of $\varphi_{\mathbf{h}}$.

(*e*) *Pseudotranslational symmetry is present*
Substructure and superstructure reflections are then described by different forms of the structure-factor equation (Böhme, 1982; Gramlich, 1984; Fan *et al.*, 1983), so that probabilistic formulae estimating triplet cosines derived on the assumption that atoms are uniformly dispersed in the unit cell cannot hold. In particular, the reliability of each triplet also depends on, besides $R_{\mathbf{h}}, R_{\mathbf{k}}, R_{\mathbf{h}-\mathbf{k}}$, the actual $\mathbf{h}$, $\mathbf{k}$, $\mathbf{h}-\mathbf{k}$ indices and on the nature of the pseudotranslation. It has been shown (Cascarano *et al.*, 1985*b*; Cascarano, Giacovazzo & Luić, 1987) that (2.2.5.7), (2.2.5.8), (2.2.5.9) still hold provided $G_{\mathbf{h},\mathbf{k}_j}$ is replaced by

$$G'_{\mathbf{h},\mathbf{k}_j} = \frac{2R_{\mathbf{h}}R_{\mathbf{k}_j}R_{\mathbf{h}-\mathbf{k}_j}}{\sqrt{N_{\mathbf{h},\mathbf{k}}}},$$

where factors E and n_i are defined according to Section 2.2.4.1,

$$N_{\mathbf{h},\mathbf{k}} = \frac{(\zeta_{\mathbf{h}}[\sigma_2]_p + [\sigma_2]_q)(\zeta_{\mathbf{k}}[\sigma_2]_p + [\sigma_2]_q)(\zeta_{\mathbf{h}-\mathbf{k}}[\sigma_2]_p + [\sigma_2]_q)}{\{(\beta/m)[\sigma_3]_p(n_1^2n_2^2n_3^2\ldots) + [\sigma_3]_q\}^2},$$

and β is the number of times for which

$$\begin{aligned} &\mathbf{h}\mathbf{R}_s\cdot\mathbf{u}_1 \equiv 0 \pmod 1 \quad \mathbf{h}\mathbf{R}_s\cdot\mathbf{u}_2 \equiv 0 \pmod 1 \quad \mathbf{h}\mathbf{R}_s\cdot\mathbf{u}_3 \equiv 0 \pmod 1 \ldots \\ &\mathbf{k}\mathbf{R}_s\cdot\mathbf{u}_1 \equiv 0 \pmod 1 \quad \mathbf{k}\mathbf{R}_s\cdot\mathbf{u}_2 \equiv 0 \pmod 1 \quad \mathbf{k}\mathbf{R}_s\cdot\mathbf{u}_3 \equiv 0 \pmod 1 \ldots \\ &(\mathbf{h}-\mathbf{k})\mathbf{R}_s\cdot\mathbf{u}_1 \equiv 0 \pmod 1 \quad (\mathbf{h}-\mathbf{k})\mathbf{R}_s\cdot\mathbf{u}_2 \equiv 0 \pmod 1 \\ &(\mathbf{h}-\mathbf{k})\mathbf{R}_s\cdot\mathbf{u}_3 \equiv 0 \pmod 1 \ldots \end{aligned}$$

are simultaneously satisfied when s varies from 1 to m. The above formulae have been generalized (Cascarano *et al.*, 1988*b*) to the case in which deviations both of replacive and of displacive type from ideal pseudo-translational symmetry occur.

2.2.5.5. *Quartet phase relationships*

In early papers (Hauptman & Karle, 1953; Simerska, 1956) the phase

$$\Phi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} - \varphi_{\mathbf{h+k+l}}$$

was always expected to be zero. Schenk (1973*a*,*b*) [see also Hauptman (1974)] suggested that Φ primarily depends on the seven magnitudes: $R_{\mathbf{h}}, R_{\mathbf{k}}, R_{\mathbf{l}}, R_{\mathbf{h+k+l}}$, called *basis magnitudes*, and $R_{\mathbf{h+k}}, R_{\mathbf{h+l}}, R_{\mathbf{k+l}}$, called *cross magnitudes.*

The conditional probability of Φ in $P1$ given seven magnitudes $(R_1 = R_{\mathbf{h}}, \ldots, R_4 = R_{\mathbf{h+k+l}}, R_5 = R_{\mathbf{h+k}}, R_6 = R_{\mathbf{h+l}}, R_7 = R_{\mathbf{k+l}})$ according to Hauptman (1975) is

$$P_7(\Phi) = \frac{1}{L}\exp(-2B\cos\Phi) I_0(2\sigma_3\sigma_2^{-3/2}R_5Y_5) \times I_0(2\sigma_3\sigma_2^{-3/2}R_6Y_6) I_0(2\sigma_3\sigma_2^{-3/2}R_7Y_7),$$

where L is a suitable normalizing constant which can be derived numerically,

$$B = \sigma_2^{-3}(3\sigma_3^2 - \sigma_2\sigma_4)R_1R_2R_3R_4$$
$$Y_5 = [R_1^2R_2^2 + R_3^2R_4^2 + 2R_1R_2R_3R_4\cos\Phi]^{1/2}$$
$$Y_6 = [R_3^2R_1^2 + R_2^2R_4^2 + 2R_1R_2R_3R_4\cos\Phi]^{1/2}$$
$$Y_7 = [R_2^2R_3^2 + R_1^2R_4^2 + 2R_1R_2R_3R_4\cos\Phi]^{1/2}.$$

For equal atoms $\sigma_2^{-3}(3\sigma_3^2 - \sigma_2\sigma_4) = 2/N$. Denoting

$$C = R_1R_2R_3R_4/N,$$
$$Z_5 = 2Y_5/\sqrt{N}, \quad Z_6 = 2Y_6/\sqrt{N}, \quad Z_7 = 2Y_7/\sqrt{N}$$

gives

$$P_7(\Phi) = \frac{1}{L}\exp(-4C\cos\Phi) \times I_0(R_5Z_5)I_0(R_6Z_6)I_0(R_7Z_7). \qquad (2.2.5.18)$$

Fig. 2.2.5.3 shows the distribution (2.2.5.18) for three typical cases. It is clear from the figure that the cosine estimated near π or in the middle range will be in poorer agreement with the true values than the cosine near 0 because of the relatively larger values of the variance. In principle, however, the formula is able to estimate negative or enantiomorph-sensitive quartet cosines from the seven magnitudes.

In the cs. case (2.2.5.18) is replaced (Hauptman & Green, 1976) by

$$P^{\pm} \simeq \frac{1}{L}\exp(\mp 2C)\cosh(R_5Z_5^{\pm}) \times \cosh(R_6Z_6^{\pm})\cosh(R_7Z_7^{\pm}), \qquad (2.2.5.19)$$

where $P^{\pm}$ is the probability that the sign of $E_1E_2E_3E_4$ is positive or negative, and

$$Z_5^{\pm} = \frac{1}{N^{1/2}}(R_1R_2 \pm R_3R_4),$$
$$Z_6^{\pm} = \frac{1}{N^{1/2}}(R_1R_3 \pm R_2R_4),$$
$$Z_7^{\pm} = \frac{1}{N^{1/2}}(R_1R_4 \pm R_2R_3).$$

The normalized probability may be derived by $P^+/(P^+ + P^-)$. More simple probabilistic formulae were derived independently by Giacovazzo (1975, 1976):

$$P_7(\Phi) = [2\pi I_0(G)]^{-1}\exp(G\cos\Phi), \qquad (2.2.5.20)$$

where

$$G = \frac{2C(1 + \varepsilon_5 + \varepsilon_6 + \varepsilon_7)}{1 + Q/(2N)} \qquad (2.2.5.21)$$

$$Q = (\varepsilon_1\varepsilon_2 + \varepsilon_3\varepsilon_4)\varepsilon_5 + (\varepsilon_1\varepsilon_3 + \varepsilon_2\varepsilon_4)\varepsilon_6 + (\varepsilon_1\varepsilon_4 + \varepsilon_2\varepsilon_3)\varepsilon_7 \qquad (2.2.5.22)$$

and $\varepsilon_i = (|E_i|^2 - 1)$. Q is never allowed to be negative.

According to (2.2.5.20) $\cos\Phi$ is expected to be positive or negative according to whether $(\varepsilon_5 + \varepsilon_6 + \varepsilon_7 + 1)$ is positive or negative: the larger is C, the more reliable is the phase indication. For $N \geq 150$, (2.2.5.18) and (2.2.5.20) are practically equivalent in all cases. If N is small, (2.2.5.20) is in good agreement with (2.2.5.18) for quartets strongly defined as positive or negative, but in poor agreement for enantiomorph-sensitive quartets (see Fig. 2.2.5.3).

In cs. cases the sign probability for $E_1E_2E_3E_4$ is

$$P^+ = \tfrac{1}{2} + \tfrac{1}{2}\tanh(G/2), \qquad (2.2.5.23)$$

where G is defined by (2.2.5.21).

All three cross magnitudes are not always in the set of measured reflections. From marginal distributions the following formulae arise (Giacovazzo, 1977*c*; Heinermann, 1977*b*):

(*a*) in the ncs. case, if R_7, or R_6 and R_7, or R_5 and R_6 and R_7, are not in the measurements, then (2.2.5.18) is replaced by

$$P(\Phi|R_1, \ldots, R_6) \simeq \frac{1}{L'}\exp(-2C\cos\Phi)I_0(R_5Z_5)I_0(R_6Z_6),$$

or

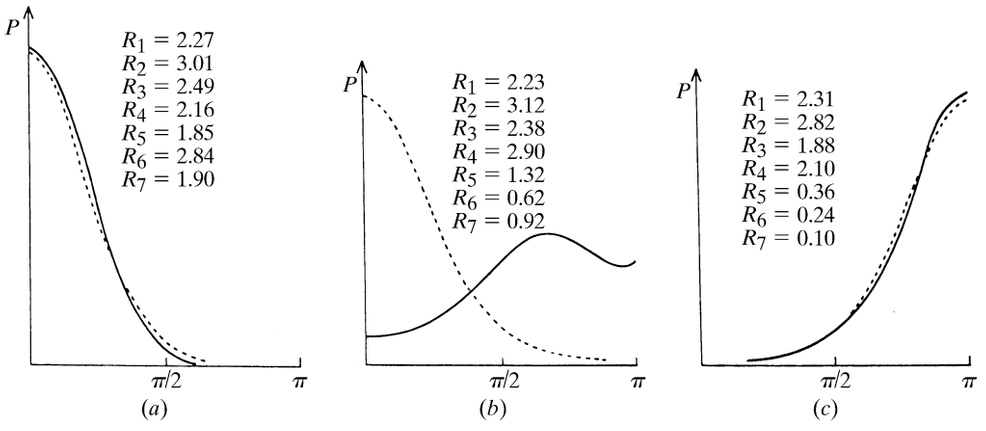

Fig. 2.2.5.3. Distributions (2.2.5.18) (——) and (2.2.5.20) (– – – –) for the indicated $|E|$ values in three typical cases.

Table 2.2.5.1. *List of quartets symmetry equivalent to* $\Phi = \Phi_1$ *in the class mmm*

Quartets	Basis vectors				Cross vectors		
Φ_1	(1, 2, 3)	$(\bar{1},5,\bar{3})$	$(\bar{1},\bar{5},8)$	$(1,\bar{2},\bar{8})$	(0, 7, 0)	$(0,\bar{3},11)$	$(\bar{2},0,5)$
Φ_2	$(\bar{1},2,3)$	$(1,5,\bar{3})$	$(\bar{1},\bar{5},8)$	$(1,\bar{2},\bar{8})$	(0, 7, 0)	$(\bar{2},\bar{3},11)$	(0, 0, 5)
Φ_3	$(1,2,\bar{3})$	$(\bar{1},5,3)$	$(\bar{1},\bar{5},8)$	$(1,\bar{2},\bar{8})$	(0, 7, 0)	$(0,\bar{3},5)$	$(\bar{2},0,11)$
Φ_4	$(\bar{1},2,\bar{3})$	(1, 5, 3)	$(\bar{1},\bar{5},8)$	$(1,\bar{2},\bar{8})$	(0, 7, 0)	$(\bar{2},\bar{3},5)$	(0, 0, 11)
Φ_5	$(\bar{1},2,3)$	$(\bar{1},5,\bar{3})$	$(1,\bar{5},8)$	$(1,\bar{2},\bar{8})$	$(\bar{2},7,0)$	$(0,\bar{3},11)$	(0, 0, 5)
Φ_6	(1, 2, 3)	$(\bar{1},\bar{5},\bar{3})$	$(\bar{1},5,8)$	$(1,\bar{2},\bar{8})$	$(0,\bar{3},0)$	(0, 7, 11)	$(\bar{2},0,5)$
Φ_7	$(\bar{1},2,3)$	$(1,\bar{5},\bar{3})$	$(\bar{1},5,8)$	$(1,\bar{2},\bar{8})$	$(0,\bar{3},0)$	$(\bar{2},7,11)$	(0, 0, 5)
Φ_8	$(\bar{1},2,\bar{3})$	$(\bar{1},5,3)$	$(1,\bar{5},8)$	$(1,\bar{2},\bar{8})$	$(\bar{2},7,0)$	$(0,\bar{3},5)$	(0, 0, 11)
Φ_9	$(1,2,\bar{3})$	$(\bar{1},\bar{5},3)$	$(\bar{1},5,8)$	$(1,\bar{2},\bar{8})$	$(0,\bar{3},0)$	(0, 7, 5)	$(\bar{2},0,11)$
Φ_{10}	$(\bar{1},2,\bar{3})$	$(1,\bar{5},3)$	$(\bar{1},5,8)$	$(1,\bar{2},\bar{8})$	$(0,\bar{3},0)$	$(\bar{2},7,5)$	(0, 0, 11)
Φ_{11}	$(\bar{1},2,3)$	$(\bar{1},\bar{5},\bar{3})$	(1, 5, 8)	$(1,\bar{2},\bar{8})$	$(\bar{2},\bar{3},0)$	(0, 7, 11)	(0, 0, 5)

$$P(\Phi|R_1,\ldots,R_5) \simeq \frac{1}{L''} I_0(R_5 Z_5),$$

or

$$P(\Phi|R_1,\ldots,R_4) \simeq \frac{1}{L'''} \exp(2C\cos\Phi),$$

respectively.

(*b*) in the same situations, we have for cs. cases

$$P^{\pm} \simeq \frac{1}{L'} \exp(\mp C)\cosh(R_5 Z_5^{\pm})\cosh(R_6 Z_6^{\pm}),$$

or

$$P^{\pm} \simeq \frac{1}{L''} \cosh(R_5 Z_5^{\pm})$$

or

$$P^{\pm} = \frac{1}{L'''} \exp(\pm C) \simeq 0.5 + 0.5\tanh(\pm C),$$

respectively.

Equations (2.2.5.20) and (2.2.5.23) are easily modifiable when some cross magnitudes are not in the measurements. If R_i is not measured then (2.2.5.20) or (2.2.5.23) are still valid provided that in G it is assumed that $\varepsilon_i = 0$. For example, if R_7 and R_6 are not in the data then (2.2.5.21) and (2.2.5.22) become

$$G = \frac{2C(1+\varepsilon_5)}{1+Q/(2N)}, \qquad Q = (\varepsilon_1\varepsilon_2 + \varepsilon_3\varepsilon_4)\varepsilon_5.$$

In space groups with symmetry higher than $P\bar{1}$ more symmetry-equivalent quartets can exist of the type

$$\psi = \varphi_{\mathbf{h}\boldsymbol{R}_\alpha} + \varphi_{\mathbf{k}\boldsymbol{R}_\beta} + \varphi_{\mathbf{l}\boldsymbol{R}_\gamma} + \varphi_{(\overline{\mathbf{h}+\mathbf{k}+\mathbf{l}})\boldsymbol{R}_\delta},$$

where $\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta, \boldsymbol{R}_\gamma, \boldsymbol{R}_\delta$ are rotation matrices of the space group. The set $\{\psi\}$ is called the *first representation* of Φ. In this case Φ primarily depends on more than seven magnitudes. For example, let us consider in *Pmmm* the quartet

$$\Phi = \varphi_{123} + \varphi_{\bar{1}5\bar{3}} + \varphi_{\bar{1}\bar{5}8} + \varphi_{1\bar{2}\bar{8}}.$$

Quartets symmetry equivalent to Φ and respective cross terms are given in Table 2.2.5.1.

Experimental tests on the application of the representation concept to quartets have recently been made (Busetta *et al.*, 1980). It was shown that quartets with more than three cross magnitudes are more accurately estimated than other quartets. Also, quartets with a cross reflection which is systematically absent were shown to be of significant importance in direct methods. In this context it is noted that systematically absent reflections are not usually included in the set of diffraction data. This custom, not exceptionable when only triplet relations are used, can give rise to a loss of information when quartets are used. In fact the usual programs of direct methods discard quartets as soon as one of the cross reflections is not measured, so that systematic absences are dealt with in the same manner as those reflections which are outside the sphere of measurements.

2.2.5.6. *Quintet phase relationships*

A quintet phase

$$\Phi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} + \varphi_{\overline{\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}}}$$

may be considered as the sum of three suitable triplets or the sum of a triplet and a quartet, *i.e.*

$$\Phi = (\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} - \varphi_{\mathbf{h}+\mathbf{k}}) + (\varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} - \varphi_{\mathbf{l}+\mathbf{m}}) + (\varphi_{\mathbf{h}+\mathbf{k}} + \varphi_{\mathbf{l}+\mathbf{m}} + \varphi_{\overline{\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}}})$$

or

$$\Phi = (\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} - \varphi_{\mathbf{h}+\mathbf{k}}) + (\varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} + \varphi_{\overline{\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}}} + \varphi_{\mathbf{h}+\mathbf{k}}).$$

It depends primarily on 15 magnitudes: the five *basis magnitudes*

$$R_{\mathbf{h}}, \quad R_{\mathbf{k}}, \quad R_{\mathbf{l}}, \quad R_{\mathbf{m}}, \quad R_{\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}},$$

and the ten *cross magnitudes*

$$R_{\mathbf{h}+\mathbf{k}}, \quad R_{\mathbf{h}+\mathbf{l}}, \quad R_{\mathbf{h}+\mathbf{m}}, \quad R_{\mathbf{k}+\mathbf{l}+\mathbf{m}}, \quad R_{\mathbf{k}+\mathbf{l}},$$
$$R_{\mathbf{k}+\mathbf{m}}, \quad R_{\mathbf{h}+\mathbf{l}+\mathbf{m}}, \quad R_{\mathbf{l}+\mathbf{m}}, \quad R_{\mathbf{h}+\mathbf{k}+\mathbf{m}}, \quad R_{\mathbf{h}+\mathbf{k}+\mathbf{l}}.$$

In the following we will denote

$$R_1 = R_{\mathbf{h}}, \quad R_2 = R_{\mathbf{k}}, \ldots, \quad R_{15} = R_{\mathbf{h}+\mathbf{k}+\mathbf{l}}.$$

Conditional distributions of Φ in $P1$ and $P\bar{1}$ given the 15 magnitudes have been derived by several authors and allow in favourable circumstances in ncs. space groups the quintets having Φ near 0 or near π or near $\pm\pi/2$ to be identified. Among others, we remember:

(*a*) the semi-empirical expression for $P_{15}(\Phi)$ suggested by Van der Putten & Schenk (1977):

$$P(\Phi|\ldots) \simeq \frac{1}{L}\exp\left[\left(6 - \sum_{j=6}^{15} R_j^2\right) 2C\cos\Phi\right] \prod_{j=6}^{15} I_0(2R_jY_j),$$

where

$$C = N^{-3/2} R_1 R_2 R_3 R_4 R_5$$

references