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The Probabilistic Theory of the Structure Invariants $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in $P1$

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Probability distributions associated with the third and fourth neighborhoods of the structure invariant $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ are described. These distributions yield estimates for the invariants φ_{lm} (not merely the cosine invariants $\cos\varphi_{lm}$) which are consistent with a specified enantiomorph. The estimates are particularly good in the favorable case that the standard deviations of the distributions are small.

1. Background

The probabilistic theory of the structure invariant

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \qquad (1.1)$$

was initiated two years ago (Hauptman, 1974*a*,*b*), and a year later (Hauptman, 1975*a*,*b*) a new method was introduced which marked a departure from earlier approaches not only for the theory of the quartet invariants (1.1) but for that of the structure invariants and seminvariants in general. The initial results strongly suggested that the value of φ_{lm} was mostly determined by one or several appropriately chosen small sets of structure factor magnitudes $|E|$, the neighborhoods of φ_{lm}. Two estimates for φ_{lm} were derived, the first dependent on the four magnitudes $|E|$ constituting the first neighborhood of φ_{lm} and the second dependent on the seven magnitudes in the second neighborhood. Finally a 'principle of nested neighborhoods' was formulated which asserted the existence of a sequence of nested neighborhoods, having increasing numbers of magnitudes, in terms of which more and more reliable estimates for φ_{lm} could be expressed.

More recently, Giacovazzo (1976) using a different mathematical formalism, obtained distributions in $P1$ associated with the seven-magnitude second neighborhood. Although superficial comparison shows qualitative agreement with the earlier results of Hauptman (1975*b*), a closer study may well reveal significant discrepancies [compare Hauptman & Green (1976) with Giacovazzo (1975) in $P\bar{1}$].

In the preceding paper (Hauptman, 1977) a sequence of nested neighborhoods was derived. In the present paper probability distributions appropriate to these higher-order neighborhoods are given, and these lead in the obvious way to estimates for φ_{lm} in terms of known magnitudes $|E|$.

Of major importance is the existence of joint conditional distributions of two or more structure invariants given magnitudes $|E|$ alone, as well as of conditional distributions of a single structure invariant, given not only magnitudes $|E|$ but also the values of one or more structure invariants. These distributions permit the estimation of the values, *i.e.* both magnitudes and signs, of a large number of structure invariants φ_{lm}, consistent with a specified enantiomorph, and not merely the estimation of the magnitudes of φ_{lm}. In this way, enantiomorph specification is made prior to the process leading from the values of the structure invariants to the values of individual phases rather than being made part of this process. In effect then, the values of both $\cos\varphi_{lm}$ and $\sin\varphi_{lm}$ are available for phase determination rather than only the values of $\cos\varphi_{lm}$, thus making the process of phase determination a better-conditioned one.

In recent work the theory was extended to cover the case of unequal atoms, in particular neutron diffraction also, since negative atomic scattering factors are permitted (Hauptman, 1976). The present paper is written from this more general point of view.

Because of their extreme length, no mathematical derivations are given here. Instead, the patterns of the earlier results are extrapolated in the obvious way and lead to estimates of the φ_{lm} which are confirmed by making application to known and unknown structures.

Next, the formulas obtained are correct to terms of order $1/N$ only, where N is the number of atoms in the unit cell. It is not yet known whether the improvement which would result if terms of order $1/N^2$ were retained justifies the enormous amount of work required to derive these more accurate distributions.

It is assumed throughout that a structure consisting of N atoms per unit cell in the space group $P1$ is fixed. The normalized structure factor $E_{\mathbf{h}}$ is defined by

$$E_{\mathbf{h}}=|E_{\mathbf{h}}|\exp(i\varphi_{\mathbf{h}})=\frac{1}{\sigma_2^{1/2}}\sum_{j=1}^{N} f_j\exp(2\pi i\mathbf{h}\,.\,\mathbf{r}_j) \qquad (1.2)$$

where f_j is the zero-angle atomic scattering factor of the atom labeled j, $\mathbf{r}_j$ is its position vector and

$$\sigma_n=\sum_{j=1}^{N} f_j^n\,. \qquad (1.3)$$

For the case of X-ray diffraction, the f_j are the atomic numbers Z_j and are therefore all positive. In the neutron diffraction case some of the f_j may be negative.

Finally, the sixfold Cartesian product $W\times W\times W$

$\times W \times W \times W$ of reciprocal space W is defined to be the collection of all ordered sextuples (**h**, **k**, **l**, **m**, **p**, **q**) of reciprocal vectors **h**, **k**, **l**, **m**, **p**, **q**; the eightfold Cartesian product $W \times W \times W \times W \times W \times W \times W \times W$ to be the collection of all ordered octuples (**h**, **k**,**l**, **m**, **p**, **q**, **r**, **s**) of reciprocal vectors **h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**, *etc.*

The third (13-magnitude) neighborhood yields three major results. (1) The joint conditional probability distribution of two quartets, given 13 magnitudes, $P_{2|13}$, equation (2.13). (2) The conditional probability distribution of a quartet, given the value of another quartet and 11 magnitudes, $P_{1|1,11}$, equation (2.33). (3) The conditional probability distribution of a quartet, given 13 magnitudes, $P_{1|13}$, equation (2.42).

The fourth (21-magnitude) neighborhood yields five major results. (1) The joint conditional probability distribution of three quartets, given 21 magnitudes, $P_{3|21}$, equation (3.22). (2) The joint conditional probability distribution of two quartets, given the value of another quartet and 19 magnitudes, $P_{2|1,19}$, equation (3.48). (3) The conditional probability distribution of a quartet, given the values of two other quartets and 15 magnitudes, $P_{1|2,15}$, equation (3.61). (4) The joint conditional probability distribution of two quartets, given 21 magnitudes, $P_{2|21}$, equation (3.72). (5) The conditional probability distribution of a quartet given 21 magnitudes, $P_{1|21}$, equation (3.73).

2. Probability distributions derived from the third (13-magnitude) neighborhoods

2.1. *Joint probability distribution of the* 13 *structure factors* $E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{p}}, E_{\mathbf{q}}; E_{\mathbf{h+k}}, E_{\mathbf{k+l}}, E_{\mathbf{l+h}}; E_{\mathbf{h+p}}, E_{\mathbf{k+p}}, E_{\mathbf{l-p}}, E_{\mathbf{m-p}}$

Refer to the preceding paper (Hauptman, 1977) for the definition of the third (13-magnitude) neighborhoods of the structure invariant

$$\varphi_{lm} = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} . \tag{2.1}$$

Suppose that the ordered sextuple (**h**, **k**, **l**, **m**, **p**, **q**) of reciprocal vectors is a random variable (vector) which is uniformly distributed over the subset of the sixfold Cartesian product $W \times W \times W \times W \times W \times W$ defined by

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0 \tag{2.2}$$

and

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0 . \tag{2.3}$$

Then the thirteen normalized structure factors $E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{p}}, E_{\mathbf{q}}; E_{\mathbf{h+k}}, E_{\mathbf{k+l}}, E_{\mathbf{l+h}}; E_{\mathbf{h+p}}, E_{\mathbf{k+p}}, E_{\mathbf{l-p}}, E_{\mathbf{m-p}}$, as functions of the primitive random variables **h**, **k**, **l**, **m**, **p**, **q**, are themselves random variables. Denote by

$$\begin{aligned} P_{13} = P(&R_1, R_2, R_3, R_4, R_5, R_6;\\ &R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, R_{3\bar{5}}, R_{4\bar{5}};\\ &\Phi_1, \Phi_2, \Phi_3, \Phi_4, \Phi_5, \Phi_6; \Phi_{12}, \Phi_{23}, \Phi_{31};\\ &\Phi_{15}, \Phi_{25}, \Phi_{3\bar{5}}, \Phi_{4\bar{5}}) \end{aligned} \tag{2.4}$$

the joint probability distribution of the magnitudes $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{p}}|, |E_{\mathbf{q}}|; |E_{\mathbf{h+k}}|, |E_{\mathbf{k+l}}|, |E_{\mathbf{l+h}}|; |E_{\mathbf{h+p}}|, |E_{\mathbf{k+p}}|, |E_{\mathbf{l-p}}|, |E_{\mathbf{m-p}}|$ and the phases $\varphi_{\mathbf{h}}, \varphi_{\mathbf{k}}, \varphi_{\mathbf{l}}, \varphi_{\mathbf{m}}, \varphi_{\mathbf{p}}, \varphi_{\mathbf{q}}; \varphi_{\mathbf{h+k}}, \varphi_{\mathbf{k+l}}, \varphi_{\mathbf{l+h}}; \varphi_{\mathbf{h+p}}, \varphi_{\mathbf{k+p}}, \varphi_{\mathbf{l-p}}, \varphi_{\mathbf{m-p}}$ of these 13 structure factors. Then, following the pattern of results recently established (Hauptman, 1975*a*, 1976), it seems clear that

$$\begin{aligned} P_{13} = &\frac{1}{\pi^{13}} R_1R_2R_3R_4R_5R_6R_{12}R_{23}R_{31}R_{15}R_{25}R_{3\bar{5}}R_{4\bar{5}}\\ &\times \exp\Big\{-R_1^2-R_2^2-R_3^2-R_4^2-R_5^2-R_6^2-R_{12}^2\\ &-R_{23}^2-R_{31}^2-R_{15}^2-R_{25}^2-R_{3\bar{5}}^2-R_{4\bar{5}}^2\\ &+\frac{2\sigma_3}{\sigma_2^{3/2}}[R_1R_2R_{12}\cos(\Phi_1+\Phi_2-\Phi_{12})\\ &+R_3R_4R_{12}\cos(\Phi_3+\Phi_4+\Phi_{12})\\ &+R_5R_6R_{12}\cos(\Phi_5+\Phi_6+\Phi_{12})\\ &+R_2R_3R_{23}\cos(\Phi_2+\Phi_3-\Phi_{23})\\ &+R_1R_4R_{23}\cos(\Phi_1+\Phi_4+\Phi_{23})\\ &+R_1R_3R_{31}\cos(\Phi_1+\Phi_3-\Phi_{31})\\ &+R_2R_4R_{31}\cos(\Phi_2+\Phi_4+\Phi_{31})\\ &+R_1R_5R_{15}\cos(\Phi_1+\Phi_5-\Phi_{15})\\ &+R_2R_6R_{15}\cos(\Phi_2+\Phi_6+\Phi_{15})\\ &+R_2R_5R_{25}\cos(\Phi_2+\Phi_5-\Phi_{25})\\ &+R_1R_6R_{25}\cos(\Phi_1+\Phi_6+\Phi_{25})\\ &+R_3R_5R_{3\bar{5}}\cos(\Phi_3-\Phi_5-\Phi_{3\bar{5}})\\ &+R_4R_6R_{3\bar{5}}\cos(\Phi_4-\Phi_6+\Phi_{3\bar{5}})\\ &+R_4R_5R_{4\bar{5}}\cos(\Phi_4-\Phi_5-\Phi_{4\bar{5}})\\ &+R_3R_6R_{4\bar{5}}\cos(\Phi_3-\Phi_6+\Phi_{4\bar{5}})]\\ &-\frac{2(3\sigma_3^2-\sigma_2\sigma_4)}{\sigma_2^3}[R_1R_2R_3R_4\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4)\\ &+R_1R_2R_5R_6\cos(\Phi_1+\Phi_2+\Phi_5+\Phi_6)\\ &+R_3R_4R_5R_6\cos(\Phi_3+\Phi_4-\Phi_5-\Phi_6)]\\ &+O\left(\frac{1}{N^{1/2}}\right)\Big\}\left\{1+O\left(\frac{1}{N}\right)\right\} \end{aligned} \tag{2.5}$$

where $O(1/N^{1/2})$ consists of all terms of order $1/N^{1/2}$ or higher in which each term of order $1/N^{1/2}$ contains three R's and three Φ's having double index and each term of order $1/N$ contains two R's and two Φ's having double index; but $O(1/N)$ consists of all terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the Φ's. It follows [refer to Hauptman (1975*b*, 1976) for details for the second neighborhood] that $O(1/N^{1/2})$ and $O(1/N)$ will make no contribution of order $1/N$ or lower to the conditional distributions derived in the sequel.

2.2. *The joint conditional probability distribution of the pair of structure invariants* $\varphi_{lm} = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}}$,

$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}$, *given the* 13 *magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$; $|E_{\mathbf{h}+\mathbf{k}}|$, $|E_{\mathbf{k}+\mathbf{l}}|$, $|E_{\mathbf{l}+\mathbf{h}}|$; $|E_{\mathbf{h}+\mathbf{p}}|$, $|E_{\mathbf{k}+\mathbf{p}}|$, $|E_{\mathbf{l}-\mathbf{p}}|$, $|E_{\mathbf{m}-\mathbf{p}}|$

Suppose that the 13 non-negative numbers R_1, R_2, R_3, R_4, R_5, R_6; R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, $R_{3\bar{5}}$, $R_{4\bar{5}}$ are specified. Assume that the ordered sextuple $(\mathbf{h}, \mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{p}, \mathbf{q})$ of reciprocal vectors is a random variable (vector) which is uniformly distributed over the subset of the sixfold Cartesian product $W\times W\times W\times W\times W\times W$ defined by

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4,\ |E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6; \tag{2.6}$$

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12},\ |E_{\mathbf{k}+\mathbf{l}}|=R_{23},\ |E_{\mathbf{l}+\mathbf{h}}|=R_{31};\ |E_{\mathbf{h}+\mathbf{p}}|=R_{15},\ |E_{\mathbf{k}+\mathbf{p}}|=R_{25},\ |E_{\mathbf{l}-\mathbf{p}}|=R_{3\bar{5}},\ |E_{\mathbf{m}-\mathbf{p}}|=R_{4\bar{5}}; \tag{2.7}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,, \tag{2.8}$$

and

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0\,. \tag{2.9}$$

In order that the domain of the primitive random variable $(\mathbf{h}, \mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{p}, \mathbf{q})$ be non-vacuous, it is necessary to interpret the equation $|E_{\mathbf{h}}|=R_1$ of (2.6), for example, as the inequalities $R_1\le|E_{\mathbf{h}}|\le R_1+\mathrm{d}R_1$ *etc.* In view of (2.8) and (2.9),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \tag{2.10}$$

and

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}} \tag{2.11}$$

are structure invariants which, as functions of the primitive random variables $\mathbf{h}$, $\mathbf{k}$, $\mathbf{l}$, $\mathbf{m}$, $\mathbf{p}$, $\mathbf{q}$, are themselves random variables. Denote by

$$P_{2|13}=P(\Phi_{34},\Phi_{56}|R_1,R_2,R_3,R_4,R_5,R_6;\ R_{12},R_{23},R_{31};\ R_{15},R_{25},R_{3\bar{5}},R_{4\bar{5}}) \tag{2.12}$$

the joint conditional probability distribution of the pair of structure invariants φ_{lm}, φ_{pq}, given the 13 magnitudes (2.6) and (2.7). Then $P_{2|13}$ is obtained from P_{13} [equation (2.5)] by fixing the 13 R's, integrating P_{13} with respect to the seven phase variables Φ_{12}, Φ_{23}, Φ_{31}; Φ_{15}, Φ_{25}, $\Phi_{3\bar{5}}$, $\Phi_{4\bar{5}}$ from 0 to 2π, and multiplying the result by a suitable normalizing parameter. [Refer to Hauptman (1975*b*, 1976), in particular Appendix III. (*D*.5) and III. (*D*.6) of the latter, for complete details for the second neighborhood.] One finally obtains, correct up to and including terms of order $1/N$,

$$\begin{aligned}P_{2|13}\simeq \frac{1}{K}\exp\{&-2B_{1234}\cos\Phi_{34}-2B_{1256}\cos\Phi_{56}-2B_{3456}\cos(\Phi_{34}-\Phi_{56})\}\\
&\times I_0\left(\frac{2\sigma_3R_{12}X'_{12}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{23}X_{23}}{\sigma_2^{3/2}}\right)\\
&\times I_0\left(\frac{2\sigma_3R_{31}X_{31}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{15}X_{15}}{\sigma_2^{3/2}}\right)\\
&\times I_0\left(\frac{2\sigma_3R_{25}X_{25}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{3\bar{5}}X_{3\bar{5}}}{\sigma_2^{3/2}}\right)\\
&\times I_0\left(\frac{2\sigma_3R_{4\bar{5}}X_{4\bar{5}}}{\sigma_2^{3/2}}\right),\end{aligned} \tag{2.13}$$

where

$$B_{1234}=\frac{3\sigma_3^2-\sigma_2\sigma_4}{\sigma_2^3}R_1R_2R_3R_4\,, \tag{2.14}$$

$$B_{1256}=\frac{3\sigma_3^2-\sigma_2\sigma_4}{\sigma_2^3}R_1R_2R_5R_6\,, \tag{2.15}$$

$$B_{3456}=\frac{3\sigma_3^2-\sigma_2\sigma_4}{\sigma_2^3}R_3R_4R_5R_6\,, \tag{2.16}$$

σ_n is defined by (1.3),

$$\begin{aligned}X'_{12}=[&R_1^2R_2^2+R_3^2R_4^2+R_5^2R_6^2\\
&+2R_1R_2R_3R_4\cos\Phi_{34}+2R_1R_2R_5R_6\cos\Phi_{56}\\
&+2R_3R_4R_5R_6\cos(\Phi_{34}-\Phi_{56})]^{1/2}\,,\end{aligned} \tag{2.17}$$

$$X_{23}=[R_2^2R_3^2+R_1^2R_4^2+2R_1R_2R_3R_4\cos\Phi_{34}]^{1/2}, \tag{2.18}$$

$$X_{31}=[R_3^2R_1^2+R_2^2R_4^2+2R_1R_2R_3R_4\cos\Phi_{34}]^{1/2}, \tag{2.19}$$

$$X_{15}=[R_1^2R_5^2+R_2^2R_6^2+2R_1R_2R_5R_6\cos\Phi_{56}]^{1/2}, \tag{2.20}$$

$$X_{25}=[R_2^2R_5^2+R_1^2R_6^2+2R_1R_2R_5R_6\cos\Phi_{56}]^{1/2}, \tag{2.21}$$

$$X_{3\bar{5}}=[R_3^2R_5^2+R_4^2R_6^2+2R_3R_4R_5R_6\cos(\Phi_{34}-\Phi_{56})]^{1/2}, \tag{2.22}$$

$$X_{4\bar{5}}=[R_4^2R_5^2+R_3^2R_6^2+2R_3R_4R_5R_6\cos(\Phi_{34}-\Phi_{56})]^{1/2}, \tag{2.23}$$

and K is a suitable normalizing parameter independent of Φ_{34} and Φ_{56} and not relevant for the present purpose. Clearly the 13 magnitudes (2.6) and (2.7) are parameters of the distribution.

In general, (2.13) has two maxima in the domain

$$-\pi<\Phi_{34}\le\pi\,, \tag{2.24}$$

$$-\pi<\Phi_{56}\le\pi\,, \tag{2.25}$$

related to each other by reflection through the origin, because (2.13) is unchanged when Φ_{34} and Φ_{56} are replaced by their negatives. One maximum yields the most probable values of the pair of invariants φ_{lm}, φ_{pq}, [(2.10) and (2.11) respectively], given the 13 magnitudes (2.6) and (2.7) for one enantiomorph, the other maximum the most probable values for the other enantiomorph. By choosing one or the other maximum, one selects the enantiomorph. In the case that the maximum occurs at $\Phi_{34}=\Phi_{56}=0$ or π, or at $\Phi_{34}=0$, $\Phi_{56}=\pi$, or at $\Phi_{34}=\pi$, $\Phi_{56}=0$, the most probable values of the pair $(\varphi_{lm}, \varphi_{pq})$ are the same for both enantiomorphs and (2.13) is not suitable for enantiomorph discrimination. It should be emphasized that when (2.13) is suitable for enantiomorph discrimination then, in general, the values (both signs and magnitudes) of two structure invariants consistent with the chosen enantiomorph are available, in contrast to the usual case when the value of only one structure invariant is used for enantiomorph selection.

2.3. *The conditional probability distribution of the structure invariant* $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, *given the value of the structure invariant* $\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ *and the* 11 *magnitudes* $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{p}}|, |E_{\mathbf{q}}|$; $|E_{\mathbf{h+k}}|, |E_{\mathbf{k+l}}|, |E_{\mathbf{l+h}}|$; $|E_{\mathbf{l-p}}|, |E_{\mathbf{m-p}}|$

Suppose that Φ_{56} $(-\pi<\Phi_{56}\le\pi)$ and the 11 non-negative numbers, $R_1, R_2, R_3, R_4, R_5, R_6; R_{12}, R_{23}, R_{31}; R_{3\bar{5}}, R_{4\bar{5}}$, are specified and that the ordered sextuple (**h**, **k**, **l**, **m**, **p**, **q**) of reciprocal vectors is the primitive random variable (vector) which is assumed to be uniformly distributed over the subset of $W\times W\times W\times W\times W\times W$ defined by

$$\varphi_{pq}=\Phi_{56}; \tag{2.26}$$

$$|E_{\mathbf{h}}|=R_1, |E_{\mathbf{k}}|=R_2, |E_{\mathbf{l}}|=R_3, |E_{\mathbf{m}}|=R_4, |E_{\mathbf{p}}|=R_5, |E_{\mathbf{q}}|=R_6; \tag{2.27}$$

$$|E_{\mathbf{h+k}}|=R_{12}, |E_{\mathbf{k+l}}|=R_{23}, |E_{\mathbf{l+h}}|=R_{31}; |E_{\mathbf{l-p}}|=R_{3\bar{5}}, |E_{\mathbf{m-p}}|=R_{4\bar{5}}; \tag{2.28}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,, \tag{2.29}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0\,. \tag{2.30}$$

In view of (2.29) and (2.30),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \tag{2.31}$$

and

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}} \tag{2.32}$$

are structure invariants. The structure invariant φ_{lm}, as a function of the primitive random variables **h**, **k**, **l**, **m**, is itself a random variable, and its conditional probability distribution, given the value of the structure invariant (2.26) and the 11 magnitudes (2.27) and (2.28), obtained from $P_{2|13}$ [equation (2.13)] by fixing Φ_{56} and multiplying by a suitable normalizing constant, is given by

$$\begin{aligned}P_{1|1,11}&=P(\Phi_{34}|\Phi_{56}; R_1, R_2, R_3, R_4, R_5, R_6; R_{12}, R_{23}, R_{31}; R_{3\bar{5}}, R_{4\bar{5}})\\&\simeq\frac{1}{L}\exp\{-2B_{1234}\cos\Phi_{34}-2B_{3456}\cos(\Phi_{34}-\Phi_{56})\}\\&\times I_0\left(\frac{2\sigma_3R_{12}X'_{12}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{23}X_{23}}{\sigma_2^{3/2}}\right)\\&\times I_0\left(\frac{2\sigma_3R_{31}X_{31}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{3\bar{5}}X_{3\bar{5}}}{\sigma_2^{3/2}}\right)\\&\times I_0\left(\frac{2\sigma_3R_{4\bar{5}}X_{4\bar{5}}}{\sigma_2^{3/2}}\right),\end{aligned} \tag{2.33}$$

where $B_{1234}, B_{3456}, X'_{12}, X_{23}, X_{31}, X_{3\bar{5}}, X_{4\bar{5}}$ are given by (2.14), (2.16), (2.17), (2.18), (2.19), (2.22), (2.23) respectively, L is a suitable normalizing parameter independent of Φ_{34}, and $\Phi_{56}, R_1, R_2, R_3, R_4, R_5, R_6; R_{12}, R_{23}, R_{31}; R_{3\bar{5}}, R_{4\bar{5}}$ are parameters of the distribution.

It should be noted that in general, *i.e.* if $\Phi_{56}\ne 0$ or π, (2.33) is not an even function of Φ_{34} and has a unique maximum in the whole interval

$$-\pi<\Phi_{34}\le\pi \tag{2.34}$$

of length 2π. In other words, once the enantiomorph has been fixed by proper choice of the value for Φ_{56}, then the most probable value (*i.e.* both sign and magnitude) for Φ_{34}, given Φ_{56} and the 11 magnitudes (2.27) and (2.28), is given by the position of the unique maximum of (2.33). The initial estimate for Φ_{56}, to be used in (2.33), in terms of magnitudes $|E|$ alone may be found, for example, from the distribution described in the following § 2.4.

If $\Phi_{56}=0$ or π then φ_{pq} has the same value for both enantiomorphs, (2.33) is an even function of Φ_{34} and, unless (2.33) has its maximum at $\Phi_{34}=0$ or π, (2.33) is bimodal, one maximum corresponding to one enantiomorph and the second to the other enantiomorph. In this case enantiomorph selection may be made by specifying arbitrarily the sign of Φ_{34} in the interval $(-\pi,\pi)$

2.4. *The conditional probability distribution of the structure invariant* $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, *given the* 13 *magnitudes* $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{p}}|, |E_{\mathbf{q}}|$; $|E_{\mathbf{h+k}}|, |E_{\mathbf{k+l}}|, |E_{\mathbf{l+h}}|$; $|E_{\mathbf{h+p}}|, |E_{\mathbf{k+p}}|, |E_{\mathbf{l-p}}|, |E_{\mathbf{m-p}}|$

Suppose that the 13 non-negative numbers $R_1, R_2, R_3, R_4, R_5, R_6; R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, R_{3\bar{5}}, R_{4\bar{5}}$ are specified and that the ordered sextuple (**h**, **k**, **l**, **m**, **p**, **q**) is the primitive random variable (vector) which is assumed to be uniformly distributed over the subset of the sixfold Cartesian product $W\times W\times W\times W\times W\times W$ defined by

$$|E_{\mathbf{h}}|=R_1, |E_{\mathbf{k}}|=R_2, |E_{\mathbf{l}}|=R_3, |E_{\mathbf{m}}|=R_4, |E_{\mathbf{p}}|=R_5, |E_{\mathbf{q}}|=R_6; \tag{2.35}$$

$$|E_{\mathbf{h+k}}|=R_{12}, |E_{\mathbf{k+l}}|=R_{23}, |E_{\mathbf{l+h}}|=R_{31}; \tag{2.36}$$

$$|E_{\mathbf{h+p}}|=R_{15}, |E_{\mathbf{k+p}}|=R_{25}, |E_{\mathbf{l-p}}|=R_{3\bar{5}}, |E_{\mathbf{m-p}}|=R_{4\bar{5}}; \tag{2.37}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,, \tag{2.38}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0\,. \tag{2.39}$$

In view of (2.38),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \tag{2.40}$$

is a structure invariant which is a function of the primitive random variables **h**, **k**, **l**, **m**. Hence φ_{lm} is itself a random variable and its conditional probability distribution

$$P_{1|13}=P(\Phi_{34}|R_1, R_2, R_3, R_4, R_5, R_6; R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, R_{3\bar{5}}, R_{4\bar{5}}), \quad (2.41)$$

given the 13 magnitudes (2.35)–(2.37), is obtained from $P_{2|13}$ [equation (2.13)] by integrating with respect to Φ_{56} from 0 to 2π:

$$P_{1|13}=\int_0^{2\pi} P_{2|13}\mathrm{d}\Phi_{56}\,. \quad (2.42)$$

Although this integration can be carried out exactly, the resulting expression is a complicated infinite multiple series which does not appear to be suitable for numerical calculation. For this reason it is suggested that the indicated integration (2.42) be carried out numerically in any given case using perhaps four or eight equal subdivisions of the interval $(0,2\pi)$.

3. Probability distributions derived from the fourth (21-magnitude) neighborhoods

Now that the pattern of probability distributions corresponding to the first three neighborhoods has been established, it is a straightforward matter to write down the analogous distributions associated with the fourth neighborhoods. These are briefly but explicitly described here in strict analogy with those of § 2.

3.1. *Joint probability distribution of the* 21 *structure factors* $E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{p}}, E_{\mathbf{q}}, E_{\mathbf{r}}, E_{\mathbf{s}}; E_{\mathbf{h+k}}, E_{\mathbf{k+l}}, E_{\mathbf{l+h}}; E_{\mathbf{h+p}}, E_{\mathbf{k+p}}, E_{\mathbf{l-p}}, E_{\mathbf{m-p}}; E_{\mathbf{h+r}}, E_{\mathbf{k+r}}, E_{\mathbf{l-r}}, E_{\mathbf{m-r}}, E_{\mathbf{p-r}}, E_{\mathbf{q-r}}$

Refer to the preceding paper (Hauptman, 1977) for the definition of the fourth (21-magnitude) neighborhoods of the structure invariant

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}\,. \quad (3.1)$$

Suppose that the ordered octuple (**h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**) of reciprocal vectors is a random variable (vector) which is uniformly distributed over the subset of the eightfold Cartesian product $W\times W\times W\times W\times W\times W \times W\times W$ defined by

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,, \quad (3.2)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0\,, \quad (3.3)$$

and

$$\mathbf{h}+\mathbf{k}+\mathbf{r}+\mathbf{s}=0\,. \quad (3.4)$$

Then the 21 normalized structure factors,

$$E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{p}}, E_{\mathbf{q}}, E_{\mathbf{r}}, E_{\mathbf{s}}; \quad (3.5)$$

$$E_{\mathbf{h+k}}, E_{\mathbf{k+l}}, E_{\mathbf{l+h}}; \quad (3.6)$$

$$E_{\mathbf{h+p}}, E_{\mathbf{k+p}}, E_{\mathbf{l-p}}, E_{\mathbf{m-p}}; \quad (3.7)$$

$$E_{\mathbf{h+r}}, E_{\mathbf{k+r}}, E_{\mathbf{l-r}}, E_{\mathbf{m-r}}, E_{\mathbf{p-r}}, E_{\mathbf{q-r}}, \quad (3.8)$$

as functions of the primitive random variables, **h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**, are themselves random variables. Denote by

$$\begin{aligned}P_{21}=P(&R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8;\\ &R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, R_{3\bar{5}}, R_{4\bar{5}};\\ &R_{17}, R_{27}, R_{3\bar{7}}, R_{4\bar{7}}, R_{5\bar{7}}, R_{6\bar{7}};\\ &\Phi_1, \Phi_2, \Phi_3, \Phi_4, \Phi_5, \Phi_6, \Phi_7, \Phi_8;\\ &\Phi_{12}, \Phi_{23}, \Phi_{31}; \Phi_{15}, \Phi_{25}, \Phi_{3\bar{5}}, \Phi_{4\bar{5}};\\ &\Phi_{17}, \Phi_{27}, \Phi_{3\bar{7}}, \Phi_{4\bar{7}}, \Phi_{5\bar{7}}, \Phi_{6\bar{7}}) \quad (3.9)\end{aligned}$$

the joint probability distribution of the magnitudes $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, \ldots$ and the phases $\varphi_{\mathbf{h}}, \varphi_{\mathbf{k}}, \ldots$ of these 21 structure factors. Then, following the pattern of the previous § 2 and recent results (Hauptman 1975*a*, 1976), one finds

$$\begin{aligned}P_{21}=&\frac{1}{\pi^{21}}R_1R_2R_3R_4R_5R_6R_7R_8R_{12}R_{23}R_{31}\\ &\times R_{15}R_{25}R_{3\bar{5}}R_{4\bar{5}}R_{17}R_{27}R_{3\bar{7}}R_{4\bar{7}}R_{5\bar{7}}R_{6\bar{7}}\\ &\times\exp(-R_1^2-R_2^2-R_3^2-R_4^2-R_5^2-R_6^2-R_7^2-R_8^2\\ &-R_{12}^2-R_{23}^2-R_{31}^2-R_{15}^2-R_{25}^2-R_{3\bar{5}}^2-R_{4\bar{5}}^2\\ &-R_{17}^2-R_{27}^2-R_{3\bar{7}}^2-R_{4\bar{7}}^2-R_{5\bar{7}}^2-R_{6\bar{7}}^2)\\ &\times\exp\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}[R_1R_2R_{12}\cos(\Phi_1+\Phi_2-\Phi_{12})\right.\\ &+R_3R_4R_{12}\cos(\Phi_3+\Phi_4+\Phi_{12})\\ &+R_5R_6R_{12}\cos(\Phi_5+\Phi_6+\Phi_{12})\\ &+R_7R_8R_{12}\cos(\Phi_7+\Phi_8+\Phi_{12})\\ &+R_2R_3R_{23}\cos(\Phi_2+\Phi_3-\Phi_{23})\\ &+R_1R_4R_{23}\cos(\Phi_1+\Phi_4+\Phi_{23})\\ &+R_1R_3R_{31}\cos(\Phi_1+\Phi_3-\Phi_{31})\\ &+R_2R_4R_{31}\cos(\Phi_2+\Phi_4+\Phi_{31})\\ &+R_1R_5R_{15}\cos(\Phi_1+\Phi_5-\Phi_{15})\\ &+R_2R_6R_{15}\cos(\Phi_2+\Phi_6+\Phi_{15})\\ &+R_2R_5R_{25}\cos(\Phi_2+\Phi_5-\Phi_{25})\\ &+R_1R_6R_{25}\cos(\Phi_1+\Phi_6+\Phi_{25})\\ &+R_3R_5R_{3\bar{5}}\cos(\Phi_3-\Phi_5-\Phi_{3\bar{5}})\\ &+R_4R_6R_{3\bar{5}}\cos(\Phi_4-\Phi_6+\Phi_{3\bar{5}})\\ &+R_4R_5R_{4\bar{5}}\cos(\Phi_4-\Phi_5-\Phi_{4\bar{5}})\\ &+R_3R_6R_{4\bar{5}}\cos(\Phi_3-\Phi_6+\Phi_{4\bar{5}})\\ &+R_1R_7R_{17}\cos(\Phi_1+\Phi_7-\Phi_{17})\\ &+R_2R_8R_{17}\cos(\Phi_2+\Phi_8+\Phi_{17})\\ &+R_2R_7R_{27}\cos(\Phi_2+\Phi_7-\Phi_{27})\\ &+R_1R_8R_{27}\cos(\Phi_1+\Phi_8+\Phi_{27})\\ &+R_3R_7R_{3\bar{7}}\cos(\Phi_3-\Phi_7-\Phi_{3\bar{7}})\\ &+R_4R_8R_{3\bar{7}}\cos(\Phi_4-\Phi_8+\Phi_{3\bar{7}})\\ &+R_4R_7R_{4\bar{7}}\cos(\Phi_4-\Phi_7-\Phi_{4\bar{7}})\\ &+R_3R_8R_{4\bar{7}}\cos(\Phi_3-\Phi_8+\Phi_{4\bar{7}})\\ &+R_5R_7R_{5\bar{7}}\cos(\Phi_5-\Phi_7-\Phi_{5\bar{7}})\end{aligned}$$

$$+R_6R_8R_{5\bar{7}}\cos(\Phi_6-\Phi_8+\Phi_{5\bar{7}})$$
$$+R_6R_7R_{6\bar{7}}\cos(\Phi_6-\Phi_7-\Phi_{6\bar{7}})$$
$$+R_5R_8R_{6\bar{7}}\cos(\Phi_5-\Phi_8+\Phi_{6\bar{7}})]$$
$$-\frac{2(3\sigma_3^2-\sigma_2\sigma_4)}{\sigma_3^2}$$
$$\times[R_1R_2R_3R_4\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4)$$
$$+R_1R_2R_5R_6\cos(\Phi_1+\Phi_2+\Phi_5+\Phi_6)$$
$$+R_1R_2R_7R_8\cos(\Phi_1+\Phi_2+\Phi_7+\Phi_8)$$
$$+R_3R_4R_5R_6\cos(\Phi_3+\Phi_4-\Phi_5-\Phi_6)$$
$$+R_3R_4R_7R_8\cos(\Phi_3+\Phi_4-\Phi_7-\Phi_8)$$
$$+R_5R_6R_7R_8\cos(\Phi_5+\Phi_6-\Phi_7-\Phi_8)]$$
$$+O\left(\frac{1}{N^{1/2}}\right)\Bigg\}\left\{1+O\left(\frac{1}{N}\right)\right\}, \qquad (3.10)$$

where $O(1/N^{1/2})$ consists of all terms of order $1/N^{1/2}$ or higher in which each term of order $1/N^{1/2}$ contains three R's and three Φ's having double index and each term of order $1/N$ contains two R's and two Φ's having double index; but $O(1/N)$ consists of all terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the Φ's. It follows [refer to Hauptman (1975*b*, 1976), in particular Appendix III of the latter reference, for details for the second neighborhood] that $O(1/N^{1/2})$ and $O(1/N)$ make no contribution of order $1/N$ or lower to the conditional probability distributions described in the sequel.

3.2. *The joint conditional probability distribution of the three structure invariants* $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, $\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}$, $\varphi_{rs}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{r}}+\varphi_{\mathbf{s}}$, *given the* 21 *magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$; $|E_{\mathbf{h+k}}|$, $|E_{\mathbf{k+l}}|$, $|E_{\mathbf{l+h}}|$; $|E_{\mathbf{h+p}}|$, $|E_{\mathbf{k+p}}|$, $|E_{\mathbf{l-p}}|$, $|E_{\mathbf{m-p}}|$; $|E_{\mathbf{h+r}}|$, $|E_{\mathbf{k+r}}|$, $|E_{\mathbf{l-r}}|$, $|E_{\mathbf{m-r}}|$, $|E_{\mathbf{p-r}}|$, $|E_{\mathbf{q-r}}|$

Suppose that the 21 non-negative numbers R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8; R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, $R_{3\bar{5}}$, $R_{4\bar{5}}$; R_{17}, R_{27}, $R_{3\bar{7}}$, $R_{4\bar{7}}$, $R_{5\bar{7}}$, $R_{6\bar{7}}$ are specified. Assume that the ordered octuple (**h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**) of reciprocal vectors is a random variable (vector) which is uniformly distributed over the subset of the eightfold Cartesian product $W\times W\times W\times W\times W\times W\times W\times W$ defined by

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4,\ |E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6,\ |E_{\mathbf{r}}|=R_7,\ |E_{\mathbf{s}}|=R_8; \qquad (3.11)$$

$$|E_{\mathbf{h+k}}|=R_{12},\ |E_{\mathbf{k+l}}|=R_{23},\ |E_{\mathbf{l+h}}|=R_{31}; \qquad (3.12)$$

$$|E_{\mathbf{h+p}}|=R_{15},\ |E_{\mathbf{k+p}}|=R_{25},\ |E_{\mathbf{l-p}}|=R_{3\bar{5}},\ |E_{\mathbf{m-p}}|=R_{4\bar{5}}; \qquad (3.13)$$

$$|E_{\mathbf{h+r}}|=R_{17},\ |E_{\mathbf{k+r}}|=R_{27},\ |E_{\mathbf{l-r}}|=R_{3\bar{7}},\ |E_{\mathbf{m-r}}|=R_{4\bar{7}},\ |E_{\mathbf{p-r}}|=R_{5\bar{7}},\ |E_{\mathbf{q-r}}|=R_{6\bar{7}}; \qquad (3.14)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0, \qquad (3.15)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0, \qquad (3.16)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{r}+\mathbf{s}=0. \qquad (3.17)$$

In view of (3.15)–(3.17),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}, \qquad (3.18)$$

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}, \qquad (3.19)$$

and

$$\varphi_{rs}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{r}}+\varphi_{\mathbf{s}} \qquad (3.20)$$

are structure invariants which, as functions of the primitive random variables **h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**, are themselves random variables. Denote by

$$P_{3|21}=P(\Phi_{34},\Phi_{56},\Phi_{78}\,|\,R_1,R_2,R_3,R_4,R_5,R_6,R_7,R_8;\ R_{12},R_{23},R_{31};R_{15},R_{25},R_{3\bar{5}},R_{4\bar{5}};\ R_{17},R_{27},R_{3\bar{7}},R_{4\bar{7}},R_{5\bar{7}},R_{6\bar{7}}) \qquad (3.21)$$

the joint conditional probability distribution of the three structure invariants φ_{lm}, φ_{pq}, φ_{rs}, given the 21 magnitudes (3.11)–(3.14). Then $P_{3|21}$ is obtained from P_{21} [equation (3.10)] by fixing the 21 R's, integrating P_{21} with respect to the 13 phase variables Φ_{12}, Φ_{23}, Φ_{31}; Φ_{15}, Φ_{25}, $\Phi_{3\bar{5}}$, $\Phi_{4\bar{5}}$; Φ_{17}, Φ_{27}, $\Phi_{3\bar{7}}$, $\Phi_{4\bar{7}}$, $\Phi_{5\bar{7}}$, $\Phi_{6\bar{7}}$ from 0 to 2π, and multiplying the result by a suitable normalizing parameter. [Refer to Hauptman (1975*b*, 1976), in particular Appendix III (*D*.5) and III (*D*.6) of the latter, for complete details for the second neighborhood.] One finally obtains, correct up to and including terms of order $1/N$,

$$P_{3|21}\simeq\frac{1}{K}\exp\{-2B_{1234}\cos\Phi_{34}-2B_{1256}\cos\Phi_{56}$$
$$-2B_{1278}\cos\Phi_{78}-2B_{3456}\cos(\Phi_{34}-\Phi_{56})$$
$$-2B_{3478}\cos(\Phi_{34}-\Phi_{78})$$
$$-2B_{5678}\cos(\Phi_{56}-\Phi_{78})\}$$
$$\times I_0\left(\frac{2\sigma_3R_{12}X_{12}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{23}X_{23}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3R_{31}X_{31}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{15}X_{15}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3R_{25}X_{25}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{3\bar{5}}X_{3\bar{5}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3R_{4\bar{5}}X_{4\bar{5}}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{17}X_{17}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3R_{27}X_{27}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{3\bar{7}}X_{3\bar{7}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3R_{4\bar{7}}X_{4\bar{7}}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{5\bar{7}}X_{5\bar{7}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3R_{6\bar{7}}X_{6\bar{7}}}{\sigma_2^{3/2}}\right), \qquad (3.22)$$

where

$$B_{\mu\nu\rho\sigma}=\frac{3\sigma_3^2-\sigma_2\sigma_4}{\sigma_2^3}R_\mu R_\nu R_\rho R_\sigma, \tag{3.23}$$

σ_n is defined by (1.3),

$$\begin{aligned}X''_{12}=[&R_1^2R_2^2+R_3^2R_4^2+R_5^2R_6^2+R_7^2R_8^2\\&+2R_1R_2R_3R_4\cos\Phi_{34}+2R_1R_2R_5R_6\cos\Phi_{56}\\&+2R_1R_2R_7R_8\cos\Phi_{78}\\&+2R_3R_4R_5R_6\cos(\Phi_{34}-\Phi_{56})\\&+2R_3R_4R_7R_8\cos(\Phi_{34}-\Phi_{78})\\&+2R_5R_6R_7R_8\cos(\Phi_{56}-\Phi_{78})]^{1/2},\end{aligned} \tag{3.24}$$

$$X_{23}=[R_2^2R_3^2+R_1^2R_4^2+2R_1R_2R_3R_4\cos\Phi_{34}]^{1/2}, \tag{3.25}$$

$$X_{31}=[R_3^2R_1^2+R_2^2R_4^2+2R_1R_2R_3R_4\cos\Phi_{34}]^{1/2}, \tag{3.26}$$

$$X_{15}=[R_1^2R_5^2+R_2^2R_6^2+2R_1R_2R_5R_6\cos\Phi_{56}]^{1/2}, \tag{3.27}$$

$$X_{25}=[R_2^2R_5^2+R_1^2R_6^2+2R_1R_2R_5R_6\cos\Phi_{56}]^{1/2}, \tag{3.28}$$

$$X_{3\bar{5}}=[R_3^2R_5^2+R_4^2R_6^2+2R_3R_4R_5R_6\cos(\Phi_{34}-\Phi_{56})]^{1/2}, \tag{3.29}$$

$$X_{4\bar{5}}=[R_4^2R_5^2+R_3^2R_6^2+2R_3R_4R_5R_6\cos(\Phi_{34}-\Phi_{56})]^{1/2}, \tag{3.30}$$

$$X_{17}=[R_1^2R_7^2+R_2^2R_8^2+2R_1R_2R_7R_8\cos\Phi_{78}]^{1/2}, \tag{3.31}$$

$$X_{27}=[R_2^2R_7^2+R_1^2R_8^2+2R_1R_2R_7R_8\cos\Phi_{78}]^{1/2}, \tag{3.32}$$

$$X_{3\bar{7}}=[R_3^2R_7^2+R_4^2R_8^2+2R_3R_4R_7R_8\cos(\Phi_{34}-\Phi_{78})]^{1/2}, \tag{3.33}$$

$$X_{4\bar{7}}=[R_4^2R_7^2+R_3^2R_8^2+2R_3R_4R_7R_8\cos(\Phi_{34}-\Phi_{78})]^{1/2}, \tag{3.34}$$

$$X_{5\bar{7}}=[R_5^2R_7^2+R_6^2R_8^2+2R_5R_6R_7R_8\cos(\Phi_{56}-\Phi_{78})]^{1/2}, \tag{3.35}$$

$$X_{6\bar{7}}=[R_6^2R_7^2+R_5^2R_8^2+2R_5R_6R_7R_8\cos(\Phi_{56}-\Phi_{78})]^{1/2}, \tag{3.36}$$

and K is a suitable normalizing parameter independent of Φ_{34}, Φ_{56} and Φ_{78} and not needed for the present purpose. Clearly the 21 magnitudes (3.11)–(3.14) are parameters of the distribution. Remarks like those in the last paragraph of § 2.2 are appropriate here too.

3.3. *The joint conditional probability distribution of the pair of structure invariants $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, $\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}$, given the value of the structure invariant $\varphi_{rs}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{r}}+\varphi_{\mathbf{s}}$ and the 19 magnitudes $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$; $|E_{\mathbf{h}+\mathbf{k}}|$, $|E_{\mathbf{k}+\mathbf{l}}|$, $|E_{\mathbf{l}+\mathbf{h}}|$; $|E_{\mathbf{h}+\mathbf{p}}|$, $|E_{\mathbf{k}+\mathbf{p}}|$, $|E_{\mathbf{l}-\mathbf{p}}|$, $|E_{\mathbf{m}-\mathbf{p}}|$; $|E_{\mathbf{l}-\mathbf{r}}|$, $|E_{\mathbf{m}-\mathbf{r}}|$, $|E_{\mathbf{p}-\mathbf{r}}|$, $|E_{\mathbf{q}-\mathbf{r}}|$*

Suppose that Φ_{78} $(-\pi<\Phi_{78}\le\pi)$ and the 19 non-negative numbers, R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8; R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, $R_{3\bar{5}}$, $R_{4\bar{5}}$; $R_{3\bar{7}}$, $R_{4\bar{7}}$, $R_{5\bar{7}}$, $R_{6\bar{7}}$, are specified and that the ordered octuple (**h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**) of reciprocal vectors is the primitive random variable which is assumed to be uniformly distributed over the subset of the eightfold Cartesian product $W\times W\times W\times W\times W\times W\times W\times W$ defined by

$$\varphi_{rs}=\Phi_{78}; \tag{3.37}$$

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4,\ |E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6,\ |E_{\mathbf{r}}|=R_7,\ |E_{\mathbf{s}}|=R_8; \tag{3.38}$$

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12},\ |E_{\mathbf{k}+\mathbf{l}}|=R_{23},\ |E_{\mathbf{l}+\mathbf{h}}|=R_{31}; \tag{3.39}$$

$$|E_{\mathbf{h}+\mathbf{p}}|=R_{15},\ |E_{\mathbf{k}+\mathbf{p}}|=R_{25},\ |E_{\mathbf{l}-\mathbf{p}}|=R_{3\bar{5}},\ |E_{\mathbf{m}-\mathbf{p}}|=R_{4\bar{5}}; \tag{3.40}$$

$$|E_{\mathbf{l}-\mathbf{r}}|=R_{3\bar{7}},\ |E_{\mathbf{m}-\mathbf{r}}|=R_{4\bar{7}},\ |E_{\mathbf{p}-\mathbf{r}}|=R_{5\bar{7}},\ |E_{\mathbf{q}-\mathbf{r}}|=R_{6\bar{7}} \tag{3.41}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0, \tag{3.42}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0, \tag{3.43}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{r}+\mathbf{s}=0. \tag{3.44}$$

In view of (3.42)–(3.44),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}, \tag{3.45}$$

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}, \tag{3.46}$$

and

$$\varphi_{rs}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{r}}+\varphi_{\mathbf{s}} \tag{3.47}$$

are structure invariants. The structure invariants φ_{lm} and φ_{pq}, as functions of the primitive random variables **h**, **k**, **l**, **m**, **p**, **q**, are themselves random variables and their joint conditional probability distribution, given the value of the structure invariant (3.37) and the 19 magnitudes (3.38)–(3.41), obtained from $P_{3|21}$ [equation (3.22)] by fixing Φ_{78} and multiplying by a suitable normalizing constant, is given by

$$\begin{aligned}P_{2|1,19}=P(&\Phi_{34},\Phi_{56}|\Phi_{78};\\&R_1,R_2,R_3,R_4,R_5,R_6,R_7,R_8;\\&R_{12},R_{23},R_{31};R_{15},R_{25},R_{3\bar{5}},R_{4\bar{5}};\\&R_{3\bar{7}},R_{4\bar{7}},R_{5\bar{7}},R_{6\bar{7}})\\\simeq\frac{1}{L}&\exp[-2B_{1234}\cos\Phi_{34}-2B_{1256}\cos\Phi_{56}\\&-2B_{3456}\cos(\Phi_{34}-\Phi_{56})\\&-2B_{3478}\cos(\Phi_{34}-\Phi_{78})\\&-2B_{5678}\cos(\Phi_{56}-\Phi_{78})]\\&\times I_0\left(\frac{2\sigma_3R_{12}X''_{12}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{23}X_{23}}{\sigma_2^{3/2}}\right)\\&\times I_0\left(\frac{2\sigma_3R_{31}X_{31}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{15}X_{15}}{\sigma_2^{3/2}}\right)\\&\times I_0\left(\frac{2\sigma_3R_{25}X_{25}}{\sigma_2^{3/2}}\right)I_0\left(\frac{2\sigma_3R_{3\bar{5}}X_{3\bar{5}}}{\sigma_2^{3/2}}\right)\end{aligned}$$

$$\times I_0\left(\frac{2\sigma_3 R_{4\bar{5}} X_{4\bar{5}}}{\sigma_2^{3/2}}\right) I_0\left(\frac{2\sigma_3 R_{3\bar{7}} X_{3\bar{7}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3 R_{4\bar{7}} X_{4\bar{7}}}{\sigma_2^{3/2}}\right) I_0\left(\frac{2\sigma_3 R_{5\bar{7}} X_{5\bar{7}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3 R_{6\bar{7}} X_{6\bar{7}}}{\sigma_2^{3/2}}\right) \quad (3.48)$$

where B_{1234}. B_{1256}, B_{3456}, B_{3478}, B_{5678}, X''_{12}, X_{23}, X_{31}, X_{15}, X_{25}, $X_{3\bar{5}}$, $X_{4\bar{5}}$, $X_{3\bar{7}}$, $X_{4\bar{7}}$, $X_{5\bar{7}}$, $X_{6\bar{7}}$ are given by (3.23)–(3.30) and (3.33)–(3.36), L is a suitable normalizing parameter independent of Φ_{34} and Φ_{56}, and Φ_{78}, R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_{12}, R_{23}, R_{31}, R_{15}, R_{25}, $R_{3\bar{5}}$, $R_{4\bar{5}}$, $R_{3\bar{7}}$, $R_{4\bar{7}}$, $R_{5\bar{7}}$, $R_{6\bar{7}}$ are parameters of the distribution.

3.4. *The conditional probability distribution of the structure invariant* $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, *given the values of the structure invariants* $\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}$, $\varphi_{rs}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{r}}+\varphi_{\mathbf{s}}$ *and the* 15 *magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$. $|E_{\mathbf{m}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$; $|E_{\mathbf{h}+\mathbf{k}}|$, $|E_{\mathbf{k}+\mathbf{l}}|$, $|E_{\mathbf{l}+\mathbf{h}}|$; $|E_{\mathbf{l}-\mathbf{p}}|$, $|E_{\mathbf{m}-\mathbf{p}}|$, $|E_{\mathbf{l}-\mathbf{r}}|$, $|E_{\mathbf{m}-\mathbf{r}}|$

Suppose that Φ_{56} $(-\pi<\Phi_{56}\le\pi)$, Φ_{78} $(-\pi<\Phi_{78}\le\pi)$ and the 15 non-negative numbers, R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8; R_{12}, R_{23}, R_{31}; $R_{3\bar{5}}$, $R_{4\bar{5}}$, $R_{3\bar{7}}$, $R_{4\bar{7}}$, are specified and that the ordered octuple (**h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**) of reciprocal vectors is the primitive random variable which is assumed to be uniformly distributed over the subset of the eightfold Cartesian product $W\times W\times W\times W\times W\times W\times W\times W$ defined by

$$\varphi_{pq}=\Phi_{56}, \quad (3.49)$$

$$\varphi_{rs}=\Phi_{78}; \quad (3.50)$$

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4,$$
$$|E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6,\ |E_{\mathbf{r}}|=R_7,\ |E_{\mathbf{s}}|=R_8; \quad (3.51)$$

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12},\ |E_{\mathbf{k}+\mathbf{l}}|=R_{23},\ |E_{\mathbf{l}+\mathbf{h}}|=R_{31}; \quad (3.52)$$

$$|E_{\mathbf{l}-\mathbf{p}}|=R_{3\bar{5}},\ |E_{\mathbf{m}-\mathbf{p}}|=R_{4\bar{5}}; \quad (3.53)$$

$$|E_{\mathbf{l}-\mathbf{r}}|=R_{3\bar{7}},\ |E_{\mathbf{m}-\mathbf{r}}|=R_{4\bar{7}}, \quad (3.54)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0, \quad (3.55)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0, \quad (3.56)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{r}+\mathbf{s}=0. \quad (3.57)$$

In view of (3.55)–(3.57),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}, \quad (3.58)$$

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}, \quad (3.59)$$

and

$$\varphi_{rs}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{r}}+\varphi_{\mathbf{s}} \quad (3.60)$$

are structure invariants. The structure invariant φ_{lm}, as a function of the primitive random variables **h**, **k**, **l**, **m**, is itself a random variable and its conditional probability distribution, given the values of the two structure invariants (3.49) and (3.50) and the 15 magnitudes (3.51)–(3.54), is obtained from $P_{3|21}$ [equation (3.22)] by fixing Φ_{56} and Φ_{78} and multiplying by a suitable normalizing constant:

$$P_{1|2,15}=P(\Phi_{34}|\Phi_{56},\Phi_{78};$$
$$R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8;$$
$$R_{12}, R_{23}, R_{31}; R_{3\bar{5}}, R_{4\bar{5}}; R_{3\bar{7}}, R_{4\bar{7}})$$
$$\simeq \frac{1}{M}\exp\{-2B_{1234}\cos\Phi_{34}$$
$$-2B_{3456}\cos(\Phi_{34}-\Phi_{56})$$
$$-2B_{3478}\cos(\Phi_{34}-\Phi_{78})\}$$
$$\times I_0\left(\frac{2\sigma_3 R_{12} X''_{12}}{\sigma_2^{3/2}}\right) I_0\left(\frac{2\sigma_3 R_{23} X_{23}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3 R_{31} X_{31}}{\sigma_2^{3/2}}\right) I_0\left(\frac{2\sigma_3 R_{3\bar{5}} X_{3\bar{5}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3 R_{4\bar{5}} X_{4\bar{5}}}{\sigma_2^{3/2}}\right) I_0\left(\frac{2\sigma_3 R_{3\bar{7}} X_{3\bar{7}}}{\sigma_2^{3/2}}\right)$$
$$\times I_0\left(\frac{2\sigma_3 R_{4\bar{7}} X_{4\bar{7}}}{\sigma_2^{3/2}}\right) \quad (3.61)$$

where B_{1234}, B_{3456}, B_{3478}, X''_{12}, X_{23}, X_{31}, $X_{3\bar{5}}$, $X_{4\bar{5}}$, $X_{3\bar{7}}$, $X_{4\bar{7}}$ are given by (3.23)–(3.26), (3.29), (3.30), (3.33), (3.34), M is a suitable normalizing parameter independent of Φ_{34}, and Φ_{56}, Φ_{78}, R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8; R_{12}, R_{23}, R_{31}; $R_{3\bar{5}}$, $R_{4\bar{5}}$, $R_{3\bar{7}}$, $R_{4\bar{7}}$ are parameters of the distribution.

3.5. *The joint conditional probability distribution of the pair of structure invariants* $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, $\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}}$, *given the* 21 *magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$; $|E_{\mathbf{h}+\mathbf{k}}|$, $|E_{\mathbf{k}+\mathbf{l}}|$, $|E_{\mathbf{l}+\mathbf{h}}|$; $|E_{\mathbf{h}+\mathbf{p}}|$, $|E_{\mathbf{k}+\mathbf{p}}|$, $|E_{\mathbf{l}-\mathbf{p}}|$, $|E_{\mathbf{m}-\mathbf{p}}|$; $|E_{\mathbf{h}+\mathbf{r}}|$, $|E_{\mathbf{k}+\mathbf{r}}|$, $|E_{\mathbf{l}-\mathbf{r}}|$, $|E_{\mathbf{m}-\mathbf{r}}|$, $|E_{\mathbf{p}-\mathbf{r}}|$, $|E_{\mathbf{q}-\mathbf{r}}|$

Suppose that the 21 non-negative numbers R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8; R_{12}, R_{23}, R_{31}; R_{15}, R_{25}, $R_{3\bar{5}}$, $R_{4\bar{5}}$; R_{17}, R_{27}, $R_{3\bar{7}}$, $R_{4\bar{7}}$, $R_{5\bar{7}}$, $R_{6\bar{7}}$ are specified and that the ordered octuple (**h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**) is the primitive random variable (vector) which is assumed to be uniformly distributed over the subset of the eightfold Cartesian product $W\times W\times W\times W\times W\times W\times W\times W$ defined by

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4,$$
$$|E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6,\ |E_{\mathbf{r}}|=R_7,\ |E_{\mathbf{s}}|=R_8; \quad (3.62)$$

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12},\ |E_{\mathbf{k}+\mathbf{l}}|=R_{23},\ |E_{\mathbf{l}+\mathbf{h}}|=R_{31}; \quad (3.63)$$

$$|E_{\mathbf{h}+\mathbf{p}}|=R_{15},\ |E_{\mathbf{k}+\mathbf{p}}|=R_{25},$$
$$|E_{\mathbf{l}-\mathbf{p}}|=R_{3\bar{5}},\ |E_{\mathbf{m}-\mathbf{p}}|=R_{4\bar{5}}; \quad (3.64)$$

$$|E_{\mathbf{h}+\mathbf{r}}|=R_{17},\ |E_{\mathbf{k}+\mathbf{r}}|=R_{27},\ |E_{\mathbf{l}-\mathbf{r}}|=R_{3\bar{7}},$$
$$|E_{\mathbf{m}-\mathbf{r}}|=R_{4\bar{7}},\ |E_{\mathbf{p}-\mathbf{r}}|=R_{5\bar{7}},\ |E_{\mathbf{q}-\mathbf{r}}|=R_{6\bar{7}}; \quad (3.65)$$

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,, \tag{3.66}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{p}+\mathbf{q}=0\,, \tag{3.67}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{r}+\mathbf{s}=0\,. \tag{3.68}$$

In view of (3.66) and (3.67),

$$\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \tag{3.69}$$

and

$$\varphi_{pq}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{p}}+\varphi_{\mathbf{q}} \tag{3.70}$$

are structure invariants which are functions of the primitive random variables **h**, **k**, **l**, **m**, **p**, **q**. Hence φ_{lm} and φ_{pq} are themselves random variables and their joint conditional probability distribution

$$P_{2|21}=P(\Phi_{34},\Phi_{56}|R_1,R_2,R_3,R_4,R_5,R_6,R_7,R_8;\; R_{12},R_{23},R_{31};R_{15},R_{25},R_{3\bar{5}},R_{4\bar{5}};\; R_{17},R_{27},R_{3\bar{7}},R_{4\bar{7}},R_{5\bar{7}},R_{6\bar{7}})\,, \tag{3.71}$$

given the 21 magnitudes (3.62)–(3.65), is obtained from $P_{3|21}$ [equation (3.22)] by integrating with respect to Φ_{78} from 0 to 2π:

$$P_{2|21}=\int_0^{2\pi} P_{3|21}\,\mathrm{d}\Phi_{78}\,. \tag{3.72}$$

Although this integration can be carried out exactly, the resulting expression appears not to be useful in the applications. For this reason it is suggested that this integration be done numerically using perhaps four or eight equal subdivisions of the interval $(0,2\pi)$ in analogy with (2.42).

3.6. *The conditional probability distribution of the structure invariant* $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, *given the* 21 *magnitudes* $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$; $|E_{\mathbf{h}+\mathbf{k}}|$, $|E_{\mathbf{k}+\mathbf{l}}|$, $|E_{\mathbf{l}+\mathbf{h}}|$; $|E_{\mathbf{h}+\mathbf{p}}|$, $|E_{\mathbf{k}+\mathbf{p}}|$, $|E_{\mathbf{l}-\mathbf{p}}|$, $|E_{\mathbf{m}-\mathbf{p}}|$; $|E_{\mathbf{h}+\mathbf{r}}|$, $|E_{\mathbf{k}+\mathbf{r}}|$, $|E_{\mathbf{l}-\mathbf{r}}|$, $|E_{\mathbf{m}-\mathbf{r}}|$, $|E_{\mathbf{p}-\mathbf{r}}|$, $|E_{\mathbf{q}-\mathbf{r}}|$

Under the same assumptions as in § 3.5, the structure invariant φ_{lm} is a random variable whose conditional probability distribution, $P_{1|21}$, given the 21 magnitudes (3.62)–(3.65), is obtained from $P_{3|21}$ by means of

$$P_{1|21}=\int_0^{2\pi}\int_0^{2\pi} P_{3|21}\,\mathrm{d}\Phi_{56}\,\mathrm{d}\Phi_{78}\,. \tag{3.73}$$

Again, the indicated double integral is best evaluated numerically subdividing the square $0\le\Phi_{56}\le 2\pi$, $0\le\Phi_{78}\le 2\pi$ into perhaps 16 or 64 sub-squares, for example.

4. Concluding remarks

Probability distributions of the structure invariant $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ corresponding to the third and fourth neighborhoods have been described. Now that the pattern of these distributions has been established, it is a straightforward matter to derive the distributions associated with the fifth (31-magnitude) and higher neighborhoods. In accordance with the principle of nested neighborhoods, it is anticipated that the distributions belonging to the higher neighborhoods will yield better estimates for the invariants and will therefore permit the determination of very complex crystal structures. Initial applications in $P\bar{1}$ confirm this prediction (Gilmore, 1976).

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