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The Probabilistic Theory of the Structure Invariants $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in $P\bar{1}$

By Herbert Hauptman

Medical Foundation of Buffalo, 73 *High Street*, *Buffalo*, *New York* 14203, *USA*

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Probability distributions associated with the third, fourth, fifth and sixth neighborhoods of the structure invariant $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ are derived. These distributions yield estimates for φ_{lm} in terms of magnitudes $|E|$ alone which are particularly good in the favorable case that the standard deviations of the distributions are small. The estimates for the φ_{lm} lead in turn to unique values for the individual phases φ even for very complex structures. Conditional distributions of φ_{lm} given the values of one or more structure invariants φ_{pq}, φ_{rs}, φ_{tu} and appropriate sets of magnitudes $|E|$ are also described.

1. Introduction

Probability distributions of the structure invariant $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ associated with the third, fourth, fifth and sixth neighborhoods (Hauptman, 1977*a*) in the space group $P\bar{1}$ are described, in strict analogy with the preceding paper in $P1$ (Hauptman, 1977*b*). Because of the heavy dependence on still earlier work (Hauptman, 1975*a*,*b*, 1976, 1977*a*; Green & Hauptman, 1976; Hauptman & Green, 1976), with which it is assumed that the reader is also familiar, the present paper is made very concise without, it is hoped, any loss of clarity. [However the long Appendices I-III, which have been deposited (see footnote on p. 567), contain many details of the derivations.]

Comparison of the present and previous work with recent results obtained by Giacovazzo (1975, 1976) is instructive particularly because of the different mathematical approaches used. Initial comparisons (Hauptman & Green, 1976) already reveal significant discrepancies so that further comparative studies, especially with respect to the applications, are called for.

2. A sequence of nested neighborhoods of the structure invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$

A sequence of nested neighborhoods of the structure invariant

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

is defined by Fig. 1 of Hauptman (1977*a*) in which it is assumed that the reciprocal vectors, **h**, **k**, **l**, **m**, **p**, **q**, **r**, **s**, **t**, **u**,... satisfy

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

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

$$\mathbf{h}+\mathbf{k}+\mathbf{r}+\mathbf{s}=0\,, \tag{2.4}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{t}+\mathbf{u}=0\,, \tag{2.5}$$

$$\mathbf{h}+\mathbf{k}+\mathbf{v}+\mathbf{w}=0\,, \tag{2.6}$$

etc., but are otherwise arbitrary (Hauptman, 1977*a*). Then φ_{lm} [equation (2.1)] is a structure invariant. A major goal of this paper is to exhibit the conditional probability distributions of φ_{lm}, given first the four magnitudes in its first neighborhood, next the seven magnitudes in its second neighborhood, then the 13 magnitudes in its third neighborhood, *etc.* Conditional distributions of φ_{lm}, given the values of one or more structure invariants as well as certain sets of magnitudes, are also described in Appendices I-III.

3. Probabilistic background and notation

It is assumed that a crystal structure in $P\bar{1}$ consisting of N atoms, not necessarily identical, in the whole unit cell is fixed, and that the four non-negative numbers R_1, R_2, R_3, R_4 are also specified. Suppose that the ordered quadruple (**h**, **k**, **l**, **m**) of reciprocal vectors is a random variable which is uniformly distributed over the subset of the fourfold Cartesian product $W\times W\times W\times W$ of reciprocal space W defined by (2.2) and

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4\,. \tag{3.1}$$

Then the structure invariant (2.1) is a random variable whose conditional probability distribution, $P_4^{\pm}$, given the four magnitudes (3.1) in its first neighborhood, depends on the parameters R_1, R_2, R_3, R_4.

If, in addition to (3.1), the three non-negative numbers R_{12}, R_{23}, R_{31} are also specified, and it is assumed that the primitive random variable (**h**, **k**, **l**, **m**) is uniformly distributed over the subset of $W\times W\times W\times W$ defined by (2.2), (3.1) and

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12},\ |E_{\mathbf{k}+\mathbf{l}}|=R_{23},\ |E_{\mathbf{l}+\mathbf{h}}|=R_{31}\,, \tag{3.2}$$

then one arrives at the conditional probability distribution, $P_7^{\pm}$, of the structure invariant φ_{lm}, given the seven magnitudes (3.1) and (3.2) in its second neighborhood.

One continues in this way first to specify the six additional non-negative numbers R_5, R_6; R_{15}, R_{25}, $R_{3\bar{5}}$, $R_{4\bar{5}}$ and then to assume that the ordered sextuple (**h**, **k**, **l**, **m**, **p**, **q**) is a random variable 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 (2.2), (2.3), (3.1), (3.2) and

$$|E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6; \tag{3.3}$$

$$|E_{\mathbf{h+p}}|=R_{15},\ |E_{\mathbf{k+p}}|=R_{25},$$
$$|E_{\mathbf{l-p}}|=R_{3\bar{5}},\ |E_{\mathbf{m-p}}|=R_{4\bar{5}}\ . \tag{3.4}$$

Now one arrives at the conditional probability distribution, $P_{13}^{\pm}$, of φ_{lm}, given the 13 magnitudes (3.1)–(3.4) in its third neighborhood.

In a similar way the conditional probability distributions, $P_{21}^{\pm}$, $P_{31}^{\pm}$, $P_{43}^{\pm}$, *etc.*, of the structure invariant φ_{lm}, given the 21, 31, 43,... magnitudes in its fourth, fifth, sixth,... neighborhoods are defined.

Denote by f_j the zero-angle atomic scattering factor of the atom labeled j and define σ_n by means of

$$\sigma_n=\sum_{j=1}^{N} f_j^n\,. \tag{3.5}$$

In the case of X-ray diffraction the f_j are equal to the atomic numbers Z_j and are therefore positive. Since the theory permits some of the f_j to be negative, the extension to the neutron diffraction case is automatic.

4. The conditional probability distributions of $\varphi_{lm}=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$

Suppose that the non-negative numbers

$$R_1,\ R_2,\ R_3,\ R_4,\ R_5,\ R_6,\ R_7,\ R_8,\ R_9,\ R_{10},\ldots; \tag{4.1}$$

$$R_{12},\ R_{23},\ R_{31}; \tag{4.2}$$

$$R_{15},\ R_{25},\ R_{3\bar{5}},\ R_{4\bar{5}}; \tag{4.3}$$

$$R_{17},\ R_{27},\ R_{3\bar{7}},\ R_{4\bar{7}},\ R_{5\bar{7}},\ R_{6\bar{7}}; \tag{4.4}$$

$$R_{19},\ R_{29},\ R_{3\bar{9}},\ R_{4\bar{9}},\ R_{5\bar{9}},\ R_{6\bar{9}},\ R_{7\bar{9}},\ R_{8\bar{9}}, \tag{4.5}$$

$$R_{1\ 11},\ R_{2\ 11},\ R_{3\ \overline{11}},\ R_{4\ \overline{11}},\ R_{5\ \overline{11}},$$
$$R_{6\ \overline{11}},\ R_{7\ \overline{11}},\ R_{8\ \overline{11}},\ R_{9\ \overline{11}},\ R_{10\ \overline{11}}; \tag{4.6}$$

are specified, that (2.2)–(2.6) are satisfied and that

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,$$
$$|E_{\mathbf{m}}|=R_4,\ |E_{\mathbf{p}}|=R_5,\ |E_{\mathbf{q}}|=R_6,$$
$$|E_{\mathbf{r}}|=R_7,\ |E_{\mathbf{s}}|=R_8,\ |E_{\mathbf{t}}|=R_9,\ |E_{\mathbf{u}}|=R_{10}\ldots, \tag{4.7}$$

$$|E_{\mathbf{h+k}}|=R_{12},\ |E_{\mathbf{k+l}}|=R_{23},\ |E_{\mathbf{l+h}}|=R_{31}; \tag{4.8}$$

$$|E_{\mathbf{h+p}}|=R_{15},\ |E_{\mathbf{k+p}}|=R_{25},$$
$$|E_{\mathbf{l-p}}|=R_{3\bar{5}},\ |E_{\mathbf{m-p}}|=R_{4\bar{5}}; \tag{4.9}$$

$$|E_{\mathbf{h+r}}|=R_{17},\ |E_{\mathbf{k+r}}|=R_{27},\ |E_{\mathbf{l-r}}|=R_{3\bar{7}},$$
$$|E_{\mathbf{m-r}}|=R_{4\bar{7}},\ |E_{\mathbf{p-r}}|=R_{5\bar{7}},\ |E_{\mathbf{q-r}}|=R_{6\bar{7}}; \tag{4.10}$$

$$|E_{\mathbf{h+t}}|=R_{19},\ |E_{\mathbf{k+t}}|=R_{29},\ |E_{\mathbf{l-t}}|=R_{3\bar{9}},$$
$$|E_{\mathbf{m-t}}|=R_{4\bar{9}},\ |E_{\mathbf{p-t}}|=R_{5\bar{9}},\ |E_{\mathbf{q-t}}|=R_{6\bar{9}},$$
$$|E_{\mathbf{r-t}}|=R_{7\bar{9}},\ |E_{\mathbf{s-t}}|=R_{8\bar{9}}; \tag{4.11}$$

etc. Define $R'_{\mu\nu}$ by means of

$$R'_{\mu\nu}=\frac{\sigma_3}{\sigma_2^{3/2}}R_{\mu\nu}\,, \tag{4.12}$$

and $B_{\mu\nu\rho\sigma}$ by

$$B_{\mu\nu\rho\sigma}=\frac{3\sigma_3^2-\sigma_2\sigma_4}{\sigma_2^3}R_\mu R_\nu R_\rho R_\sigma\,, \tag{4.13}$$

where σ_n is given by (3.5).

Denote by $P_4^{\pm}$, $P_7^{\pm}$, $P_{13}^{\pm}$,... the conditional probability that

$$\cos\varphi_{lm}=\pm 1\,, \tag{4.14}$$

given the 4, 7, 13,... magnitudes in the first, second, third,... neighborhoods of φ_{lm}. Then

$$P_\mu^{\pm}=\frac{1}{K_\mu}Z_\mu^{\pm},\ \mu=4,\,7,\,13,\ldots, \tag{4.15}$$

where

$$K_\mu=Z_\mu^{+}+Z_\mu^{-}\,, \tag{4.16}$$

$$Z_4^{\pm}=\exp\left(\pm\frac{\sigma_4}{\sigma_2^2}R_1R_2R_3R_4\right) \tag{4.17}$$

$$Z_7^{\pm}=M^{\pm}A^{\pm}\,, \tag{4.18}$$

$$Z_{13}^{\pm}=M^{\pm}(A_1^{\pm}+A_2^{\pm})\,, \tag{4.19}$$

$$Z_{21}^{\pm}=M^{\pm}[M_1^{\pm}(A_{11}^{\pm}+A_{12}^{\pm})+M_2^{\pm}(A_{21}^{\pm}+A_{22}^{\pm})]\,, \tag{4.20}$$

$$\begin{aligned}Z_{31}^{\pm}=M^{\pm}\{&M_1^{\pm}[M_{11}^{\pm}(A_{111}^{\pm}+A_{112}^{\pm})\\&+M_{12}^{\pm}(A_{121}^{\pm}+A_{122}^{\pm})]\\&+M_2^{\pm}[M_{21}^{\pm}(A_{211}^{\pm}+A_{212}^{\pm})\\&+M_{22}^{\pm}(A_{221}^{\pm}+A_{222}^{\pm})]\}\,,\end{aligned} \tag{4.21}$$

$$\begin{aligned}Z_{43}^{\pm}=M^{\pm}\{&M_1^{\pm}[M_{11}^{\pm}(M_{111}^{\pm}\{A_{1111}^{\pm}+A_{1112}^{\pm}\}\\&+M_{112}^{\pm}\{A_{1121}^{\pm}+A_{1122}^{\pm}\})\\&+M_{12}^{\pm}(M_{121}^{\pm}\{A_{1211}^{\pm}+A_{1212}^{\pm}\}\\&+M_{122}^{\pm}\{A_{1221}^{\pm}+A_{1222}^{\pm}\})]\\&+M_2^{\pm}[M_{21}^{\pm}(M_{211}^{\pm}\{A_{2111}^{\pm}+A_{2112}^{\pm}\}\\&+M_{212}^{\pm}\{A_{2121}^{\pm}+A_{2122}^{\pm}\})\\&+M_{22}^{\pm}(M_{221}^{\pm}\{A_{2211}^{\pm}+A_{2212}^{\pm}\}\\&+M_{222}^{\pm}\{A_{2221}^{\pm}+A_{2222}^{\pm}\})]\}\,,\end{aligned} \tag{4.22}$$

etc.,

$$\begin{aligned}M^{\pm}=\exp(\mp B_{1234})\cosh&[R'_{23}(R_2R_3\pm R_1R_4)]\\&\times\cosh[R'_{31}(R_3R_1\pm R_2R_4)]\,,\end{aligned} \tag{4.23}$$

$$\begin{aligned}M_\mu^{\pm}=\exp&[(-1)^\mu B_{1256}\pm(-1)^\mu B_{3456}]\\&\times\cosh[R'_{15}(R_1R_5-(-1)^\mu R_2R_6)]\\&\times\cosh[R'_{25}(R_2R_5-(-1)^\mu R_1R_6)]\\&\times\cosh[R'_{3\bar{5}}(R_3R_5\mp(-1)^\mu R_4R_6)]\\&\times\cosh[R'_{4\bar{5}}(R_4R_5\mp(-1)^\mu R_3R_6)]\,,\end{aligned}$$
$$\mu=1,\,2, \tag{4.24}$$

$$
\begin{aligned}
M^{\pm}_{\mu\nu} = & \exp\,[(-1)^{\nu}B_{1278} \pm (-1)^{\nu}B_{3478} - (-1)^{\mu+\nu}B_{5678}] \\
& \times \cosh\,[R'_{17}(R_1R_7 - (-1)^{\nu}R_2R_8)] \\
& \times \cosh\,[R'_{27}(R_2R_7 - (-1)^{\nu}R_1R_8)] \\
& \times \cosh\,[R'_{3\bar{7}}(R_3R_7 \mp (-1)^{\nu}R_4R_8)] \\
& \times \cosh\,[R'_{4\bar{7}}(R_4R_7 \mp (-1)^{\nu}R_3R_8)] \\
& \times \cosh\,[R'_{5\bar{7}}(R_5R_7 + (-1)^{\mu+\nu}R_6R_8)] \\
& \times \cosh\,[R'_{6\bar{7}}(R_6R_7 + (-1)^{\mu+\nu}R_5R_8)]\,, \\
& \mu = 1, 2;\ \nu = 1, 2,
\end{aligned} \tag{4.25}
$$

$$
\begin{aligned}
M^{\pm}_{\mu\nu\rho} = & \exp\,[(-1)^{\rho}B_{1\,2\,9\,10} \pm (-1)^{\rho}B_{3\,4\,9\,10} \\
& - (-1)^{\mu+\rho}B_{5\,6\,9\,10} - (-1)^{\nu+\rho}B_{7\,8\,9\,10}] \\
& \times \cosh\,[R'_{19}(R_1R_9 - (-1)^{\rho}R_2R_{10})] \\
& \times \cosh\,[R'_{29}(R_2R_9 - (1)^{\rho}R_1R_{10})] \\
& \times \cosh\,[R'_{3\bar{9}}(R_3R_9 \mp (-1)^{\rho}R_4R_{10})] \\
& \times \cosh\,[R'_{4\bar{9}}(R_4R_9 \mp (-1)^{\rho}R_3R_{10})] \\
& \times \cosh\,[R'_{5\bar{9}}(R_5R_9 + (-1)^{\mu+\rho}R_6R_{10})] \\
& \times \cosh\,[R'_{6\bar{9}}(R_6R_9 + (-1)^{\mu+\rho}R_5R_{10})] \\
& \times \cosh\,[R'_{7\bar{9}}(R_7R_9 + (-1)^{\nu+\rho}R_8R_{10})] \\
& \times \cosh\,[R'_{8\bar{9}}(R_8R_9 + (-1)^{\nu+\rho}R_7R_{10})]\,, \\
& \mu = 1, 2;\ \nu = 1, 2;\ \rho = 1, 2,
\end{aligned} \tag{4.26}
$$

$$
\begin{aligned}
M^{\pm}_{\mu\nu\rho\sigma} = & \exp\,[(-1)^{\sigma}B_{1\,2\,11\,\underline{12}} \\
& \pm (-1)^{\sigma}B_{3\,4\,11\,\underline{12}} - (-1)^{\mu+\sigma}B_{5\,6\,11\,\underline{12}} \\
& - (-1)^{\nu+\sigma}B_{7\,8\,11\,\underline{12}} - (-1)^{\rho+\sigma}B_{9\,10\,11\,\underline{12}}] \\
& \times \cosh\,[R'_{1\,11}(R_1R_{11} - (-1)^{\sigma}R_2R_{\underline{12}})] \\
& \times \cosh\,[R'_{2\,11}(R_2R_{11} - (-1)^{\sigma}R_1R_{\underline{12}})] \\
& \times \cosh\,[R'_{3\,\overline{11}}(R_3R_{11} \mp (-1)^{\sigma}R_4R_{\underline{12}})] \\
& \times \cosh\,[R'_{4\,\overline{11}}(R_4R_{11} \mp (-1)^{\sigma}R_3R_{\underline{12}})] \\
& \times \cosh\,[R'_{5\,\overline{11}}(R_5R_{11} + (-1)^{\mu+\sigma}R_6R_{\underline{12}})] \\
& \times \cosh\,[R'_{6\,\overline{11}}(R_6R_{11} + (-1)^{\mu+\sigma}R_5R_{\underline{12}})] \\
& \times \cosh\,[R'_{7\,\overline{11}}(R_7R_{11} + (-1)^{\nu+\sigma} + R_8R_{\underline{12}})] \\
& \times \cosh\,[R'_{8\,\overline{11}}(R_8R_{11} + (-1)^{\nu+\sigma}R_7R_{\underline{12}})] \\
& \times \cosh\,[R'_{9\,\overline{11}}(R_9R_{11} + (-1)^{\rho+\sigma} + R_{10}R_{\underline{12}})] \\
& \times \cosh\,[R'_{10\,\overline{11}}(R_{10}R_{11} + (-1)^{\rho+\sigma}R_9R_{\underline{12}})]\,, \\
& \mu = 1, 2;\ \nu = 1, 2;\ \rho = 1, 2;\ \sigma = 1, 2,
\end{aligned} \tag{4.27}
$$

etc. [note that the notation $|E_{\mathbf{w}}| = R_{\underline{12}}$ is introduced in order to avoid confusion with (4.8) in which $|E_{\mathbf{h}+\mathbf{k}}| = R_{12}$],

$$A^{\pm} = \cosh\,[R'_{12}(R_1R_2 \pm R_3R_4)]\,, \tag{4.28}$$

$$
\begin{aligned}
A^{\pm}_{\mu} = & M^{\pm}_{\mu} \cosh\,[R'_{12}(R_1R_2 \pm R_3R_4 - (-1)^{\mu}R_5R_6)]\,, \\
& \mu = 1, 2,
\end{aligned} \tag{4.29}
$$

$$
\begin{aligned}
A^{\pm}_{\mu\nu} = & M^{\pm}_{\mu\nu} \cosh\,[R'_{12}(R_1R_2 \pm R_3R_4 \\
& - (-1)^{\mu}R_5R_6 - (-1)^{\nu}R_7R_8)]\,, \\
& \mu = 1, 2;\ \nu = 1, 2,
\end{aligned} \tag{4.30}
$$

$$
\begin{aligned}
A^{\pm}_{\mu\nu\rho} = & M^{\pm}_{\mu\nu\rho} \cosh\,[R'_{12}(R_1R_2 \pm R_3R_4 \\
& - (-1)^{\mu}R_5R_6 - (-1)^{\nu}R_7R_8 - (-1)^{\rho}R_9R_{10})]\,, \\
& \mu = 1, 2;\ \nu = 1, 2;\ \rho = 1, 2,
\end{aligned} \tag{4.31}
$$

$$
\begin{aligned}
A^{\pm}_{\mu\nu\rho\sigma} = & M^{\pm}_{\mu\nu\rho\sigma} \cosh\,[R'_{12}(R_1R_2 \pm R_3R_4 \\
& - (-1)^{\mu}R_5R_6 - (-1)^{\nu}R_7R_8 - (-1)^{\rho}R_9R_{10} \\
& - (-1)^{\sigma}R_{11}R_{\underline{12}}]\,, \\
& \mu = 1, 2;\ \nu = 1, 2;\ \rho = 1, 2;\ \sigma = 1, 2,
\end{aligned} \tag{4.32}
$$

etc.

Finally the variance of the distribution (4.15) is given by

$$s^2_{\mu} = 4P^+_{\mu}P^-_{\mu} = \frac{4Z^+_{\mu}Z^-_{\mu}}{(Z^+_{\mu} + Z^-_{\mu})^2}, \quad \mu = 4, 7, 13, \ldots . \tag{4.33}$$

The cases $\mu = 4$ and 7 of (4.15) have been derived previously (Hauptman & Green, 1976). The cases $\mu = 13$, 21 and 31 are described in the Appendices I, II and III respectively* [equations (I.49)–(I.54); (II.93)–(II.102); (III.64)–(III.81) respectively]. In addition, these Appendices contain many related distributions, *e.g.* the joint conditional probability distributions of two or more structure invariants, given certain sets of magnitudes, the conditional distributions of a single structure invariant, given the values of one or more structure invariants and appropriate sets of magnitudes, *etc.* which, it is anticipated, will play an important role in procedures of phase determination.

Initial applications of the formulas derived here have already been made (Gilmore, 1976; Kruger, Green, Langs & Weeks, 1976) and confirm the expectation that, at least up to and including the third neighborhoods, the higher neighborhoods do in fact yield more reliable estimates for the quartets.

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* Appendices I, II, and III have been deposited with the British Lending Library Division as Supplementary Publication No. SUP 32462 (80 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England, or from the author.

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Quintets: a Sequence of Nested Neighborhoods of the Structure Invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$

BY HERBERT HAUPTMAN

Medical Foundation of Buffalo, 73 *High Street*, *Buffalo*, *New York* 14203, *USA*

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A sequence of nested neighborhoods of the structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$ is derived. Each neighborhood is a subset of the succeeding ones and consists of the small number of structure factor magnitudes $|E|$ upon which, in favorable cases, the value of φ mostly depends.

1. Introduction

Although the neighborhood concept was introduced only a year ago (Hauptman, 1975*a*, *b*), its important role in identifying the small set of magnitudes $|E|$ on which the value of a given structure invariant or seminvariant φ mostly depends is now firmly established (Hauptman, 1976; Green & Hauptman, 1976). In the present paper a sequence of nested neighborhoods of the five-phase structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$ is obtained. In subsequent work the related probability distributions are derived, and these in turn lead to explicit estimates for φ in terms of magnitudes $|E|$. In the accompanying papers (Fortier & Hauptman, 1977; Hauptman & Fortier, 1977) the conditional probability distribution of φ, given the 15 magnitudes in the second neighborhood, is derived for the space group $P1$.

2. The first neighborhood

Let **h**, **k**, **l**, **m**, **n** be reciprocal vectors which satisfy

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=0\,. \tag{2.1}$$

Then the linear combination of phases

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}} \tag{2.2}$$

is a structure invariant. In analogy with earlier work (Hauptman, 1975*a*, *b*) the first neighborhood of φ is defined to consist of the five magnitudes

$$|E_{\mathbf{h}}|,\ |E_{\mathbf{k}}|,\ |E_{\mathbf{l}}|,\ |E_{\mathbf{m}}|,\ |E_{\mathbf{n}}|, \tag{2.3}$$

shown schematically as the first shell in Fig. 1. [Also see Schenk (1975) for the identity of the first two neighborhoods.]

3. The second neighborhood

Assume that the six magnitudes

$$|E_{\mathbf{h}}|,\ |E_{\mathbf{k}}|,\ |E_{\mathbf{l}}|,\ |E_{\mathbf{m}}|,\ |E_{\mathbf{n}}|,\ |E_{\mathbf{h}+\mathbf{k}}| \tag{3.1}$$

are all large. Then it is known that the structure invariant

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h}-\mathbf{k}}\simeq 0\,. \tag{3.2}$$

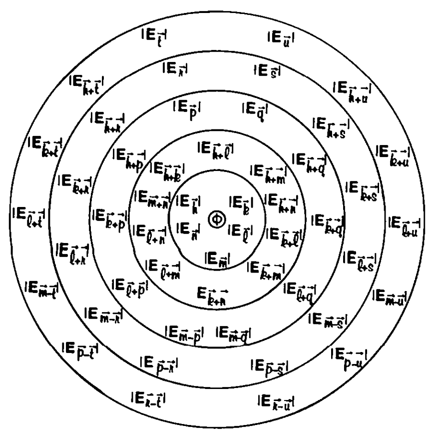

Fig. 1. A sequence of nested neighborhoods for the five-phase structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$. The reciprocal vectors **h**, **k**, **l**, **m**, **n**, **p**, **q**, **r**, **s**, **t**, **u** satisfy $\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{p}+\mathbf{q}=\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{r}+\mathbf{s}=\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{t}+\mathbf{u}=0$, but are otherwise arbitrary. In the applications it is best that $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{n}}|$, $|E_{\mathbf{p}}|$, $|E_{\mathbf{q}}|$, $|E_{\mathbf{r}}|$, $|E_{\mathbf{s}}|$, $|E_{\mathbf{t}}|$, $|E_{\mathbf{u}}|$ be large.