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Pairs in $P2_1$: Probability Distributions which Lead to Estimates of the Two-Phase Structure Seminvariants in the Vicinity of $\pm\pi/2$

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The second sequence of nested neighborhoods of the two-phase structure seminvariant $\varphi_{12} - \varphi_{h_1kl_2} - \varphi_{h_1kl_2}$ in the space group $P2_1$ is defined, and conditional probability distributions associated with the first four neighborhoods derived. In the favorable case that the variance of a distribution happens to be small, the distribution yields a particular reliable value for φ_{12}. The most reliable estimates are obtained when $\varphi_{12} \simeq \pm\pi/2$, thus facilitating enantiomorph specification in this space group.

1. Introduction

In the space group $P2_1$ the linear combination of two phases

$$\varphi_{12} = \varphi_{h_1kl_1} - \varphi_{h_2kl_2} \tag{1.1}$$

is a structure seminvariant if and only if

$$(h_1 - h_2, 0, l_1 - l_2) \equiv 0 (\mathrm{mod}\ \omega_s) \tag{1.2}$$

where ω_s, the seminvariant modulus in $P2_1$, is defined by

$$\omega_s = (2,0,2). \tag{1.3}$$

Following the first paper in this series (Green & Hauptman, 1978*a*), the probabilistic theory of this two-phase structure seminvariant is developed further *via* the Principle of Nested Neighborhoods (Hauptman, 1975*a*,*b*). The neighborhoods to be studied here, the second sequence, contain elements different from those of the first sequence derived in the previous paper and are called neighborhoods of the second kind. In sharp contrast to the relatively unreliable estimate $\pm\pi/2$ for φ_{12} obtainable from the neighborhoods of the first sequence, the most reliable estimates obtainable from the second sequence of neighborhoods are those in the vicinity of $\pm\pi/2$. Thus the present work complements the results of the previous paper and facilitates enantiomorph specification as well.

2. The second sequence of neighborhoods of the two-phase structure seminvariant $\varphi_{h_1kl_1} - \varphi_{h_2kl_2}$ in $P2_1$

2.1. *The first neighborhood*

Construct the four-phase structure invariant

$$\varphi_{h_1kl_1} - \varphi_{h_2kl_2} + \varphi_{h_1kl_1} - \varphi_{h_2kl_2}. \tag{2.1}$$

The symmetry in $P2_1$ enables one to write (2.1) as

$$2(\varphi_{h_1kl_1} - \varphi_{h_2kl_2}) \tag{2.2}$$

which is a structure seminvariant in this space group since

$$2[(h_1 - h_2). 0, (l_1 - l_2)] \equiv 0 \ (\mathrm{mod}\ \omega_s). \tag{2.3}$$

In view of the theory of the first neighborhood of the four-phase structure invariant (Hauptman, 1975*a*,*b*), it follows that if the two magnitudes

$$|E_{h_1kl_1}|, |E_{h_2kl_2}| \tag{2.4}$$

are large, then

$$2\varphi_{12} \simeq 0 \tag{2.5}$$

or

$$\varphi_{12} \simeq 0,\pi. \tag{2.6}$$

Equation (2.6) implies that both values $0,\pi$, of φ_{12} are equally probable. The first neighborhood of φ_{12} of the second kind is then defined to consist of the two magnitudes (2.4), shown as the first shell of Fig. 1.

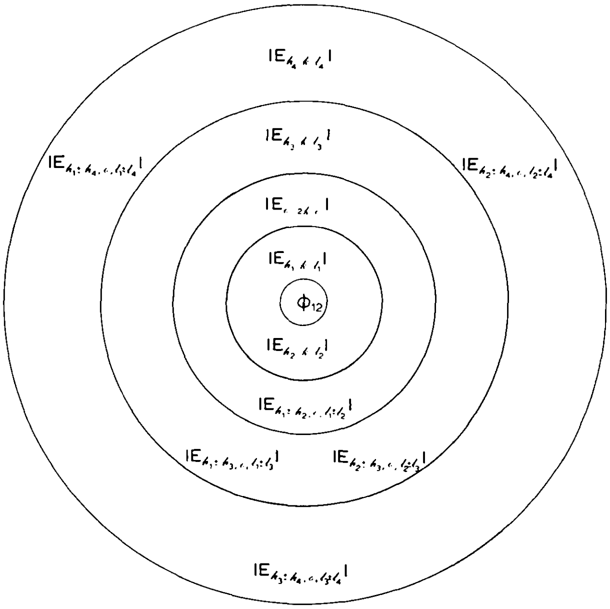

Fig. 1. The second sequence of nested neighborhoods of the two-phase structure seminvariant φ_{12} in $P2_1$; $h_\mu \equiv h_\nu$ (mod 2) and $l_\mu \equiv l_\nu$ (mod 2). The first neighborhood consists of the two magnitudes in the first shell, the second neighborhood of the five magnitudes in the first two shells, *etc.*

2.2. *The second neighborhood*

Employing the second neighborhood of the quartet theory (Hauptman, 1975*a*,*b*), the second neighborhood of φ_{12} is defined to consist of the two magnitudes in (2.4) and the three additional magnitudes

$$|E_{02k0}|, \quad |E_{h_1+h_2,0,l_1+l_2}|, \quad |E_{h_1-h_2,0,l_1-l_2}|, \tag{2.7}$$

shown in the second shell of Fig. 1. Again, from the quartet theory, if the five magnitudes of the second neighborhood are large,

$$\varphi_{12} \simeq 0,\pi \tag{2.8}$$

with high reliability, but with minimal useful phase information because of the twofold ambiguity. However, if the two magnitudes (2.4) are large and the three magnitudes in (2.7) are small then

$$2\varphi_{12} \simeq \pi \tag{2.9}$$

and

$$\varphi_{12} \simeq \pm\pi/2. \tag{2.10}$$

In contrast to the estimate (2.8) of φ_{12}, which is ambiguous, the estimate $+\pi/2$ of (2.10) corresponds to one enantiomorph and the estimate $-\pi/2$ corresponds to the other enantiomorph. Thus the second neighborhood has the potential to permit the identification of those two-phase seminvariants whose values are likely to be $\pm\pi/2$ and are therefore enantiomorph sensitive.

2.3. *The third neighborhood*

The magnitudes of the third neighborhood are constructed by arguments similar to those in the preceding paper (Green & Hauptman, 1978*a*) and for the third neighborhood of the quartet (Hauptman, 1977*a*). The construction of the two two-phase seminvariants

$$\varphi_{23} = \varphi_{h_2kl_2} - \varphi_{h_3kl_3}, \tag{2.11}$$

$$\varphi_{31} = \varphi_{h_3kl_3} - \varphi_{h_1kl_1}, \tag{2.12}$$

each having a five-magnitude second neighborhood similar to (2.4) and (2.7), leads to the identity

$$\varphi_{12} + \varphi_{23} + \varphi_{31} \equiv 0. \tag{2.13}$$

Only 10 of the 15 magnitudes forming the three corresponding second neighborhoods are distinct; they are, in addition to the five magnitudes (2.4) and (2.7) of the second neighborhood, the five magnitudes

$$\begin{aligned}&|E_{h_3kl_3}|, \quad |E_{h_2+h_3,0,l_2+l_3}|, \quad |E_{h_3+h_1,0,l_3+l_1}|,\\ &|E_{h_2-h_3,0,l_2-l_3}|, \quad |E_{h_3-h_1,0,l_3-l_1}|,\end{aligned} \tag{2.14}$$

shown in the third shell of Fig. 1.

2.4. *The fourth neighborhood*

In view of the previously referenced work, the identity of the fourth neighborhood follows from the 10 magnitudes of the third neighborhood and the 15 magnitudes obtained from the five-magnitude second neighborhoods of the three additional two-phase seminvariants:

$$\varphi_{14} = \varphi_{h_1kl_1} - \varphi_{h_4kl_4} \tag{2.15}$$

$$\varphi_{42} = \varphi_{h_4kl_4} - \varphi_{h_2kl_2} \tag{2.16}$$

$$\varphi_{43} = \varphi_{h_4kl_4} - \varphi_{h_3kl_3}. \tag{2.17}$$

In this way one is led to the 17 magnitudes of the fourth neighborhood of φ_{12}, the ten magnitudes (2.4), (2.7), (2.14) and the seven additional magnitudes

$$\begin{aligned}&|E_{h_4kl_4}|, \quad |E_{h_1+h_4,0,l_1+l_4}|, \quad |E_{h_1-h_4,0,l_1-l_4}|,\\ &|E_{h_4+h_2,0,l_4+l_2}|, \quad |E_{h_4+h_3,0,l_4+l_3}|,\\ &|E_{h_4-h_2,0,l_4-l_2}|, \quad |E_{h_4-h_3,0,l_4-l_3}|,\end{aligned} \tag{2.18}$$

shown in the fourth shell of Fig. 1. Associated with this 17-magnitude fourth neighborhood are the three identities, (2.13),

$$\varphi_{23} + \varphi_{34} + \varphi_{42} \equiv 0, \tag{2.19}$$

and

$$\varphi_{31} + \varphi_{14} + \varphi_{43} \equiv 0. \tag{2.20}$$

The last two identities are obtained by combining (2.15)–(2.17) with (2.11) and (2.12).

3. Probabilistic background and notation

Fix the 17 non-negative numbers R_1, R_2, R_3, R_4, R_0, R_{12}, $R_{1\bar{2}}$, R_{23}, $R_{2\bar{3}}$, R_{31}, $R_{3\bar{1}}$, R_{14}, $R_{1\bar{4}}$, R_{42}, $R_{4\bar{2}}$, R_{43}, $R_{4\bar{3}}$ such that

$$|E_{h_1kl_1}| = R_1, \quad |E_{h_2kl_2}| = R_2, \tag{3.1}$$

$$\begin{aligned}&|E_{02k0}| = R_0, \quad |E_{h_1+h_2,0,l_1+l_2}| = R_{12},\\ &|E_{h_1-h_2,0,l_1-l_2}| = R_{1\bar{2}},\end{aligned} \tag{3.2}$$

$$\begin{aligned}&|E_{h_3kl_3}| = R_3, \quad |E_{h_2+h_3,0,l_2+l_3}| = R_{23},\\ &|E_{h_2-h_3,0,l_2-l_3}| = R_{2\bar{3}},\\ &|E_{h_3+h_1,0,l_3+l_1}| = R_{31}, \quad |E_{h_3-h_1,0,l_3-l_1}| = R_{3\bar{1}},\end{aligned} \tag{3.3}$$

$$\begin{aligned}&|E_{h_4kl_4}| = R_4, \quad |E_{h_1+h_4,0,l_1+l_4}| = R_{14},\\ &|E_{h_1-h_4,0,l_1-l_4}| = R_{1\bar{4}}, \quad |E_{h_4+h_2,0,l_4+l_2}| = R_{42},\\ &|E_{h_4-h_2,0,l_4-l_2}| = R_{4\bar{2}},\\ &|E_{h_4+h_3,0,l_4+l_3}| = R_{43}, \quad |E_{h_4-h_3,0,l_4-l_3}| = R_{4\bar{3}}.\end{aligned} \tag{3.4}$$

Assume that a crystal structure in $P2_1$ consisting of N atoms, not necessarily identical, in the unit cell is fixed, and that the ordered pair $[(h_1kl_1), (h_2kl_2)]$ of reciprocal vectors is a random variable uniformly distributed over that subset of the twofold Cartesian product $W \times W$ of reciprocal space defined by (1.2), (1.3) and (3.1). Then the structure seminvariant, φ_{12}, is a random variable whose conditional probability distribution, $P_{1|2}$, given the two magnitudes (3.1) in its first neighborhood, depends on the parameters R_1, R_2.

If it is assumed that the primitive random variable $[(h_1kl_1), (h_2kl_2)]$ is uniformly distributed over the subset of $W \times W$ defined by (1.2), (1.3), (3.1) and (3.2), then one is led to the conditional probability distribution, $P_{1|5}$, of φ_{12}, given the five magnitudes in its second neighborhood.

One continues in this way to specify the five additional non-negative numbers R_3, R_{23}, R_{31}, $R_{2\bar{3}}$, $R_{3\bar{1}}$ and then to assume that the ordered triple $[(h_1kl_1), (h_2kl_2), (h_3kl_3)]$ is a random variable (vector) which is uniformly distributed over the subset of the threefold Cartesian product $W \times W \times W$ defined by (1.2)

$$(h_2-h_3, 0, l_2-l_3) \equiv 0 \pmod{\omega_s}, \qquad (3.5)$$

$$(h_3-h_1, 0, l_3-l_1) \equiv 0 \pmod{\omega_s}, \qquad (3.6)$$

and (3.1)–(3.3). This leads to the conditional probability distribution $P_{1|10}$, of φ_{12}, given the 10 magnitudes (3.1)–(3.3) in its third neighborhood. In a similar way, one arrives at the conditional probability distribution of φ_{12}, $P_{1|17}$, given the 17 magnitudes (3.1)–(3.4) in its fourth neighborhood.

In $P2_1$ the normalized structure factor E_{hkl} is defined by

$$E_{hkl} = |E_{hkl}| \exp(i\varphi_{hkl})$$

$$= \frac{2}{(\varepsilon\sigma_2)^{1/2}} \sum_{j=1}^{N/2} f_j \cos 2\pi\left(\mathbf{h}.\mathbf{r}_j + \frac{k}{4}\right)$$

$$\times \exp\left[2\pi i\left(ky_j - \frac{k}{4}\right)\right] \qquad (3.7)$$

where $\mathbf{h}$ and $\mathbf{r}_j$ are two-dimensional vectors defined by

$$\mathbf{h} = (h,l), \qquad (3.8)$$

$$\mathbf{r}_j = (x_j,z_j) \qquad (3.9)$$

and f_j is the zero-angle atomic scattering factor of the atom labeled j; for X-ray diffraction the f_j are the atomic numbers Z_j and are therefore positive; in the neutron diffraction case some of the f_j may be negative; the term σ_n is defined by

$$\sigma_n = \sum_{j=1}^{N} f_j^n, \qquad (3.10)$$

and $\varepsilon = 2$ if $h = l = 0$ and 1 for all other values of h and l. Finally, (x_j,y_j,z_j) is the position vector of the jth atom.

In the sequel conditional probability distributions of φ_{12}, given the magnitudes in each of its first four neighborhoods, are described. A brief account of the analysis is given in Appendix I only for the typical case of the second neighborhood, and familiarity with earlier work is assumed [*e.g.* Hauptman (1977*b*,*c*)].

4. The conditional probability distribution of the two-phase structure seminvariant $\varphi_{12} = \varphi_{h_1kl_1} - \varphi_{h_2kl_2}$, given the two magnitudes in its first neighborhood

Suppose that the two non-negative numbers R_1,R_2 defined by (3.1) are specified. Then, complete to terms of order $1/N$, the conditional probability distribution of φ_{12}, given the two magnitudes (3.1) in the first neighborhood, $P_{1|2} = P(\Phi|R_1,R_2)$, is found to be

$$P_{1|2} = \frac{1}{2\pi I_0\left(\frac{\sigma_4}{\sigma_2^2} R_1^2R_2^2\right)} \exp\left\{\frac{\sigma_4}{\sigma_2^2} R_1^2R_2^2 \cos 2\Phi\right\}. \qquad (4.1)$$

5. The conditional probability distribution of φ_{12}, given the five magnitudes in its second neighborhood

Assume that the five non-negative numbers defined by (3.1), (3.2) are specified. Then, complete to terms of order $1/N$, the conditional probability distribution, $P_{1|5}$, of φ_{12}, given the five magnitudes of the second neighborhood is

$$P_{1|5} = \frac{1}{K_{1|5}} \exp\left\{-\left(\frac{4\sigma_3^2 - \sigma_2\sigma_4}{\sigma_2^3}\right) R_1^2R_2^2 \cos 2\Phi\right\}$$

$$\times I_0\left\{\frac{2^{3/2}\sigma_3R_0}{\sigma_2^{3/2}} [R_1^4 + R_2^4 + 2R_1^2R_2^2 \cos 2\Phi]^{1/2}\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}} R_1R_2R_{12} \cos \Phi\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}} R_1R_2R_{1\bar{2}} \cos \Phi\right\}. \qquad (5.1)$$

The normalization factor $K_{1|5}$ is easily obtained by numerical techniques. Details of the derivation of (5.1) are given in Appendix I.*

6. The conditional probability distribution of φ_{12}, given the 10 magnitudes in its third neighborhood

One continues in this way to specify the 10 non-negative numbers defined by (3.1)–(3.3). Then, $P_{1|10}$, the conditional probability distribution of φ_{12} given the 10 magnitudes in the third neighborhood, is found to be

$$P_{1|10} \simeq \frac{1}{K_{1|10}} Q_1(\Phi) \int_{\Phi_{23}=0}^{2\pi} Q_2(\Phi,\Phi_{23})\, I_0\left\{\frac{2^{3/2}\sigma_3R_0}{\sigma_2^{3/2}}\right.$$

$$\times [R_1^4 + R_2^4 + R_3^4 + 2R_1^2R_2^2 \cos 2\Phi$$

$$+ 2R_2^2R_3^2 \cos 2\Phi_{23}$$

$$\left. + 2R_3^2R_1^2 \cos 2(\Phi + \Phi_{23})]^{1/2}\right\} d\Phi_{23}, \qquad (6.1)$$

* Appendix I has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32950 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

where

$$Q_1(\Phi) = \exp\left\{-\left(\frac{4\sigma_3^2 - \sigma_2\sigma_4}{\sigma_2^3}\right)R_1^2R_2^2\cos 2\Phi\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_1R_2R_{12}\cos\Phi\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_1R_2R_{1\bar{2}}\cos\Phi\right\}, \tag{6.2}$$

$$\Phi_2(\Phi,\Phi_{23}) = \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_2R_3R_{23}\cos\Phi_{23}\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_2R_3R_{2\bar{3}}\cos\Phi_{23}\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_3R_1R_{31}\cos(\Phi+\Phi_{23})\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_3R_1R_{3\bar{1}}\cos(\Phi+\Phi_{23})\right\}. \tag{6.3}$$

Following the derivation of $P_{1|15}$ in the previous paper (Green & Hauptman, 1978*a*) one may use numerical techniques to evaluate the integral in (6.1) or approximate the integrand by a suitable function; in either case the integration leads to a function of order $1/N^2$. Therefore, $P_{1|10}$ contains all terms of order $1/N$ plus those terms of order $1/N^2$ which reflect the identity (2.13).

7. The conditional probability distribution of φ_{12}, given the 17 magnitudes in its fourth neighborhood

Denote by $P_{1|17}$ the conditional probability distribution of φ_{12}, given the 17 magnitudes in the fourth neighborhood defined by (3.1)–(3.4). Then

$$P_{1|17} \simeq \frac{1}{K_{1|17}}\, Q_1(\Phi) \int\limits_{\Phi_{23}=0}^{2\pi} Q_2(\Phi,\Phi_{23}) \int\limits_{\Phi_{14}=0}^{2\pi} Q_3(\Phi,\Phi_{23},\Phi_{14})$$

$$\times I_0\left\{\frac{2^{3/2}\sigma_3R_0}{\sigma_2^{3/2}}\,[R_1^4 + R_2^4 + R_3^4 + R_4^4 + 2R_1^2R_2^2\cos 2\Phi\right.$$

$$+ 2R_2^2R_3^2\cos 2\Phi_{23} + 2R_3^2R_1^2\cos 2(\Phi+\Phi_{23})$$

$$+ 2R_1^2R_4^2\cos 2\Phi_{14} + 2R_4^2R_2^2\cos 2(\Phi-\Phi_{14})$$

$$\left. + 2R_4^2R_3^2\cos 2(\Phi+\Phi_{23}-\Phi_{14})]^{1/2}\right\}\mathrm{d}\Phi_{14}\mathrm{d}\Phi_{23}, \tag{7.1}$$

where $Q_1(\Phi)$ and $Q_2(\Phi,\Phi_{23})$ are given by (6.2) and (6.3), and

$$Q_3(\Phi,\Phi_{23},\Phi_{14}) = \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_1R_4R_{41}\cos\Phi_{14}\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_1R_4R_{1\bar{4}}\cos\Phi_{14}\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_4R_2R_{42}\cos(\Phi-\Phi_{14})\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_4R_2R_{4\bar{2}}\cos(\Phi-\Phi_{14})\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_4R_3R_{43}\cos(\Phi+\Phi_{23}-\Phi_{14})\right\}$$

$$\times \cosh\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}R_4R_3R_{4\bar{3}}\cos(\Phi+\Phi_{23}-\Phi_{14})\right\}. \tag{7.2}$$

The integration of (7.1) leads to an expression for $P_{1|17}$ which contains terms of order $1/N^2$ reflecting the information content of the identities (2.13), (2.19), (2.20).

8. The applications

The accompanying Figs. 2–6 show $P_{1|2}$, $P_{1|5}$, $P_{1|10}$, and $P_{1|17}$ as functions of Φ in the interval $-180° \le \Phi \le +180°$. They illustrate the properties of these probability distributions for a structure containing $N = 100$

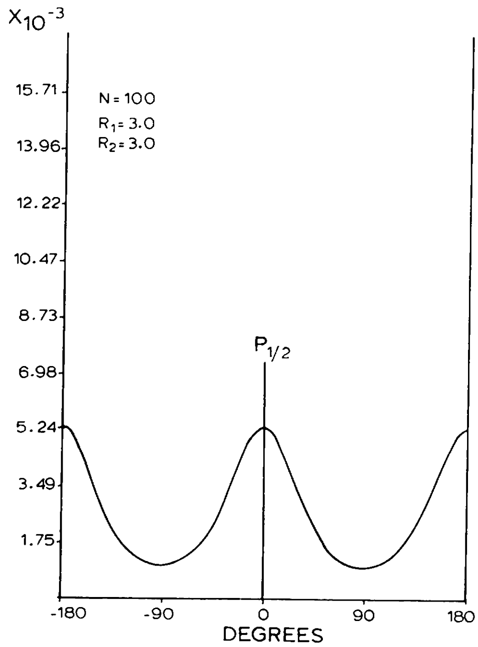

Fig. 2. The distribution $P_{1|2}$ for the values of the parameters shown.

identical atoms in the unit cell. The values selected for the magnitudes exemplify ideal behavior of these distributions by minimizing the variance and show the gains which the higher neighborhoods have the potential to yield. Fig. 2 shows that, for structures of this complexity, the first neighborhood is incapable of yielding a reliable estimate for φ_{12}. The distribution is always bimodal, with maxima at 0 and 180°, and a variance too large to yield a reliable, but ambiguous estimate. Figs. 3 and 4 illustrate the two types of reliable estimates for φ_{12} based on the five magnitudes of the second neighborhood. If the five magnitudes (3.1), (3.2) are large (Fig. 3), the most probable value of φ_{12} is 0 or 180°, and the distribution yields a reliable, but ambiguous, estimate. If the two magnitudes (3.1)

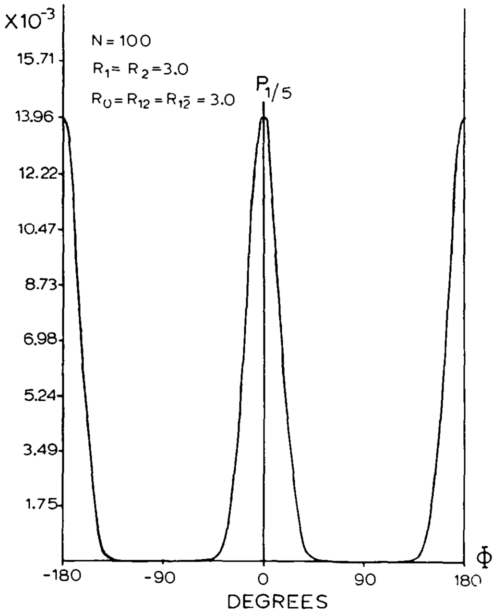

Fig. 3. The distribution $P_{1|5}$ for the values of the parameters shown.

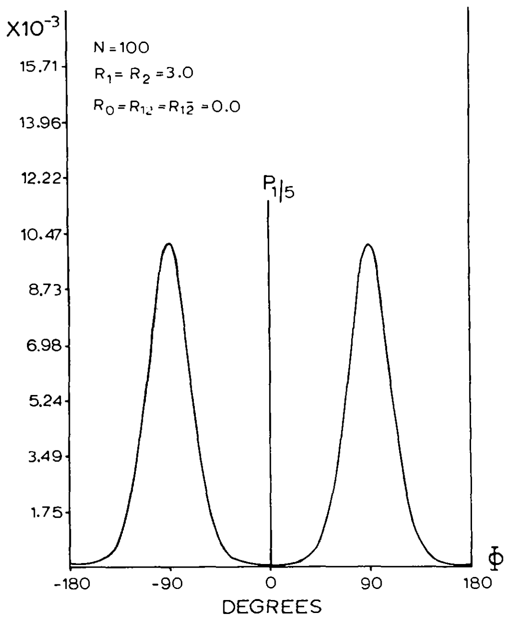

Fig. 4. The distribution $P_{1|5}$ for the values of the parameters shown.

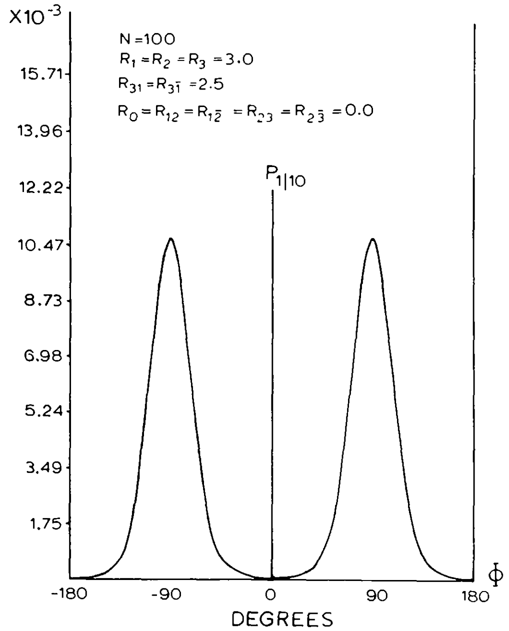

Fig. 5. The distribution $P_{1|10}$ for the values of the parameters shown.

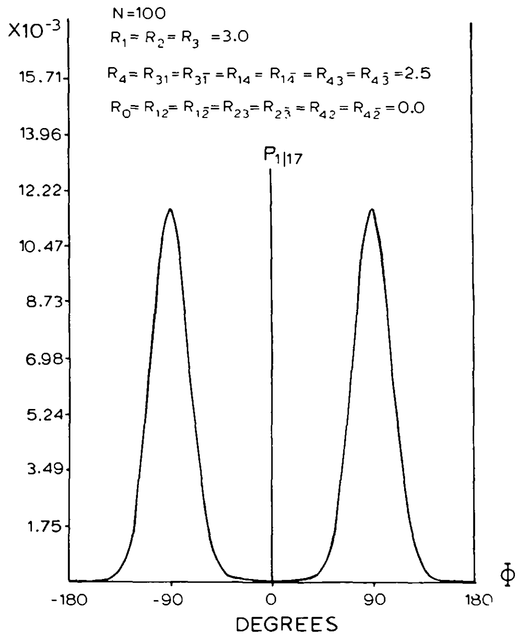

Fig. 6. The distribution $P_{1|17}$ for the values of the parameters shown.

are large but the three magnitudes (3.2) are small (Fig. 4), then a reliable estimate of φ_{12} equal to $\pm 90°$ is obtained. By selecting either value, the enantiomorph is specified.

Figs. 5 and 6 show that as the size of the neighborhood is increased there is a greater potential for obtaining a more reliable estimate for φ_{12}. Since all distributions are bimodal, only those are illustrated in Figs. 5 and 6 with maxima at $\pm 90°$ because in this case the distribution yields a unique estimate of φ_{12}, a consequence of the enantiomorph selecting capability of such a distribution. As will be shown in the following paper (Green & Hauptman, 1978*b*) the ability to identify those seminvariants having values near $\pm 90°$ leads to a procedure for eliminating the twofold ambiguity in these reliably estimated seminvariants so that unique values for many two-phase seminvariants, consistent with the specified enantiomorph, are obtained.

9. Concluding remarks

The second sequence of nested neighborhoods of the two-phase structure seminvariant in $P2_1$ has been found. The conditional probability distributions of φ_{12}, given, first, the two magnitudes in the first neighborhood; next, the five magnitudes of the second neighborhood; then the 10 magnitudes of the third neighborhood; and finally, the 17 magnitudes in the fourth neighborhood, have been derived. The distributions yield estimates for φ_{12} which may lie anywhere in the interval $(-\pi, \pi)$, but which are most useful in the case that $\varphi_{12} \simeq \pm\pi/2$ because then the estimates are among the most reliable and the resolution of the twofold ambiguity is equivalent to choosing the enantiomorph. In the accompanying paper (Green & Hauptman, 1978*b*) the question of the consistent resolution of the ambiguity for many (enantiomorph sensitive) seminvariants is addressed. It is observed again that, as more magnitudes are used, more reliable estimates for φ_{12} are obtainable (*cf.* Fig. 2, having a relatively large variance, with Figs. 3–6 where the variances are small), although, for the values of the parameters shown, the improvement in $P_{1|10}$ and $P_{1|17}$ over $P_{1|5}$ is only marginal.

Finally, the first application of the results derived here has been made to the determination of an unknown structure which had resisted solution by standard techniques (Duchamp, 1977).

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