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A Heuristic Study of Neighborhoods of the Structure Seminvariants in the Space Group $P\bar{1}$

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The first two neighborhoods of each of the structure seminvariants $\varphi_{\mathbf{h}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in the space group $P\bar{1}$ are found. Not only do these neighborhoods identify the magnitudes of the normalized structure factors $|E|$ most intimately related to the value of the associated structure seminvariant, but the analysis suggests in a qualitative way what the nature of this relation must be. Thus the stage is set for determining the conditional probability distribution of a structure seminvariant, given the magnitudes $|E|$ of a corresponding neighborhood (or an appropriate subset), and this leads in turn to a probabilistic estimate for the seminvariant in terms of a suitably chosen small set of magnitudes.

I. Introduction

In recent work (Hauptman, 1974*a*, *b*; 1975*a*, *b*) the probabilistic theory of the four-phase structure invariants in $P1$,

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}\,, \tag{1.1}$$

where

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,, \tag{1.2}$$

was initiated. The chief result was the derivation of the conditional probability distributions of φ, given, in the first instance, the four magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}| \tag{1.3}$$

and, in the second instance, the seven magnitudes consisting of those in (1.3) and the three additional magnitudes

$$|E_{\mathbf{h}+\mathbf{k}}|, |E_{\mathbf{k}+\mathbf{l}}|, |E_{\mathbf{l}+\mathbf{h}}|\,. \tag{1.4}$$

I. 1. *The neighborhood concept*

It has been known for many years that the magnitudes of the structure factors uniquely determine in general (*i.e.* if no homometric structures, other than enantiomorphs, exist) the values of the cosine invariants. The results described in the preceding paragraph suggest a sharpening of this view by means of the concept of the 'neighborhood of a structure invariant' which has recently been formulated (Hauptman, 1975*b*). Thus the first neighborhood of the structure invariant (1.1) consists of the four magnitudes (1.3), the second neighborhood consists of the seven magnitudes (1.3) and (1.4), *etc.* In this way one obtains a 'sequence of nested neighborhoods', each contained within the succeeding one, and having the property that the cosine invariants cos φ may be estimated in terms of the magnitudes constituting any neighborhood of φ (the 'principle of nested neighborhoods'). In short, the value of cosφ is approximated by means of the magnitudes 'in the neighborhood' of φ (interpolation point of view). Naturally, one anticipates that, in general, the more magnitudes used the better the approximation, 'in the probabilistic sense', *i.e.* with more magnitudes the greater the potential that the corresponding conditional distribution of φ has a small variance, and for such invariants the approximation is particularly good. In summary then, the value of the cosine invariant is mostly dependent on the values of one or more small sets of appropriately chosen magnitudes and is relatively insensitive to the values of the vast bulk of the remaining magnitudes.

If the results obtained for the structure invariant (1.1) are to carry over to the structure seminvariants in general, it is clear that an essential intermediate goal is to identify the neighborhoods of the structure seminvariants in all the space groups. The remainder of this paper is devoted to the determination of the initial neighborhoods (and their critical subsets) for each of the structure seminvariants $\varphi_{\mathbf{h}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in the space group $P\bar{1}$.

II. The one-phase structure seminvariant, $\varphi_{\mathbf{h}}$, in $P\bar{1}$

In the space group $P\bar{1}$ the single phase

$$\varphi_{\mathbf{h}} \tag{2.1}$$

is a structure seminvariant if and only if

$$\mathbf{h}\equiv 0 \pmod{\boldsymbol{\omega}_s} \tag{2.2}$$

where $\boldsymbol{\omega}_s$, the seminvariant modulus, is the three-dimensional vector defined by

$$\boldsymbol{\omega}_s=(2,2,2)\,. \tag{2.3}$$

In short, $\varphi_{\mathbf{h}}$ is a structure seminvariant if and only if the three components of $\mathbf{h}$ are even integers.

II. 1. *The first neighborhood*

Assume that (2.2) holds so that the components of $\mathbf{h}/2$ are integers. Construct the structure invariant

$$\varphi_{\mathbf{h}}+\varphi_{-\mathbf{h}/2}+\varphi_{-\mathbf{h}/2} \tag{2.4}$$

and suppose the two magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{h}/2}| \tag{2.5}$$

are very large. Under these circumstances it is known (2.4) is equal to 0 with high probability. In $P\bar{1}$ every phase is 0 or π. Hence, if both magnitudes (2.5) are large, (2.4) implies $\varphi_{\mathbf{h}}=0$ with high probability, *i.e.*

$$\varphi_{\mathbf{h}} \simeq 0\,, \tag{2.6}$$

and the larger the values of the two magnitudes (2.5) the more likely it is that (2.6) holds. The first neighborhood of $\varphi_{\mathbf{h}}$ is therefore defined to be the set of two magnitudes (2.5). Since one cannot determine the value of $\varphi_{\mathbf{h}}$ with high probability unless $|E_{\mathbf{h}}|$ is large, it is plausible to conjecture that

$$\varphi_{\mathbf{h}} \simeq \pi \tag{2.7}$$

if $|E_{\mathbf{h}}|$ is large and $|E_{\mathbf{h}/2}|$ is small.

II. 2. *The second neighborhood(s)*

Construct the two structure invariants

$$\varphi_{\mathbf{h}} + \varphi_{-(\mathbf{h}/2)-\mathbf{r}} + \varphi_{-(\mathbf{h}/2)+\mathbf{r}} \tag{2.8}$$

$$\varphi_{(\mathbf{h}/2)+\mathbf{r}} + \varphi_{-(\mathbf{h}/2)+\mathbf{r}} + \varphi_{-\mathbf{r}} + \varphi_{-\mathbf{r}} \tag{2.9}$$

where $\mathbf{r}$ is an arbitrary reciprocal vector. Then it is known (Hauptman & Green, 1976), provided the four magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{r}}|, |E_{(\mathbf{h}/2)\pm\mathbf{r}}| \tag{2.10}$$

are all large, (2.8) is probably 0 and (2.9) is probably 0 or π according as the two magnitudes

$$|E_{\mathbf{h}/2}|, |E_{2\mathbf{r}}| \tag{2.11}$$

are both large or both small respectively. Every phase in $P\bar{1}$ is equal to 0 or π. Hence, by addition of (2.8) to (2.9), it follows, if all four magnitudes of (2.10) are large, $\varphi_{\mathbf{h}}$ is probably 0 or π according as the magnitudes (2.11) are both large or both small respectively. Therefore the second neighborhood(s) of the structure seminvariant $\varphi_{\mathbf{h}}$ is (are) defined to be the set(s) of six magnitudes (2.10) and (2.11), where $\mathbf{r}$ is an arbitrary reciprocal vector. The results secured here are summarized schematically by means of Fig. 1 and Table 1.

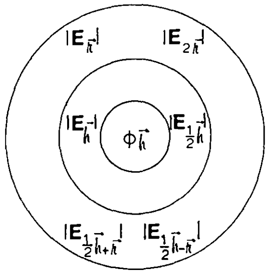

Fig. 1. The first two neighborhoods of the structure seminvariant $\varphi_{\mathbf{h}}$ in $P\bar{1}$. Here $\mathbf{r}$ may be arbitrary, but in order to obtain the most reliable estimates for $\varphi_{\mathbf{h}}$, it is best that $|E_{\mathbf{h}}|$, $|E_{\mathbf{r}}|$ and $|E_{(\mathbf{h}/2)\pm\mathbf{r}}|$ be mostly large. (See Table 1.)

Table 1. *The probable values of the structure seminvariant $\varphi_{\mathbf{h}}$ in $P\bar{1}$, given the values of the six magnitudes in its second neighborhood*

Here and in the following tables L means large and S means small.

	Magnitudes $\|E\|$					
$\varphi_{\mathbf{h}}$	$\mathbf{h}$	$\mathbf{h}/2$	$\mathbf{r}$	$2\mathbf{r}$	$(\mathbf{h}/2)+\mathbf{r}$	$(\mathbf{h}/2)-\mathbf{r}$
0	L	L	L	L	L	L
π	L	S	L	S	L	L

III. The two-phase structure seminvariant, $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$, in $P\bar{1}$

In the space group $P\bar{1}$ the linear combination of two phases

$$\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} \tag{3.1}$$

is a structure seminvariant if and only if

$$\mathbf{h}+\mathbf{k} \equiv 0 \ (\mathrm{mod}\ \boldsymbol{\omega}_s) \tag{3.2}$$

where $\boldsymbol{\omega}_s$, the seminvariant modulus, is defined by (2.3). In other words, $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ is a structure seminvariant if and only if the three components of the reciprocal vector $\mathbf{h}+\mathbf{k}$ are even.

III. 1. *The first neighborhood*

Assume that (3.2) holds so that the components of each of $(\mathbf{h}\pm\mathbf{k})/2$ are integers. Construct the two structure invariants

$$\varphi_{\mathbf{h}} + \varphi_{-(\mathbf{h}+\mathbf{k})/2} + \varphi_{-(\mathbf{h}-\mathbf{k})/2}\,, \tag{3.3}$$

$$\varphi_{\mathbf{k}} + \varphi_{-(\mathbf{h}+\mathbf{k})/2} + \varphi_{(\mathbf{h}-\mathbf{k})/2}\,. \tag{3.4}$$

Suppose further the four magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{(\mathbf{h}\pm\mathbf{k})/2}| \tag{3.5}$$

are very large. Under these circumstances it is known that each of (3.3), (3.4) is equal to 0 with high probability. In $P\bar{1}$ every phase is 0 or π. Hence, if the four magnitudes (3.5) are large, (3.3) and (3.4) imply, by addition, $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}=0$ with high probability, *i.e.*

$$\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} \simeq 0\,, \tag{3.6}$$

and the larger the values of the four magnitudes (3.5) the more likely it is that (3.6) holds. The first neighborhood of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ is therefore defined to be the set of four magnitudes (3.5). [Although this kind of argument has already been given by Grant, Howells & Rogers (1957) in their description of the coincidence method, it is the neighborhood concept which makes the extension described in the sequel seem so natural and the evidence so compelling.] Since one cannot determine the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ with high probability unless $|E_{\mathbf{h}}|$ and $|E_{\mathbf{k}}|$ are both large, it follows $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}=\pi$ with high probability only if at least one of $|E_{(\mathbf{h}\pm\mathbf{k}/2)}|$ is small. This result is refined in the next section.

III. 2. *The second neighborhood*

Construct the structure invariant

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{-(\mathbf{h}+\mathbf{k})/2}+\varphi_{-(\mathbf{h}+\mathbf{k})/2}\,. \tag{3.7}$$

Then it is known (Hauptman & Green, 1976) that, provided the three magnitudes

$$|E_{\mathbf{h}}|,|E_{\mathbf{k}}|,|E_{(\mathbf{h}+\mathbf{k})/2}| \tag{3.8}$$

are all large, the value of the structure invariant (3.7) is probably 0 or π according as the magnitudes

$$|E_{\mathbf{h}+\mathbf{k}}|,|E_{(\mathbf{h}-\mathbf{k})/2}| \tag{3.9}$$

are both large or both small respectively. However, since the space group is $P\bar{1}$, the sum of the last two terms of (3.7) is 0. Hence, provided first that the three magnitudes (3.8) are all large, it follows that

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}\simeq 0 \text{ or } \pi \tag{3.10}$$

according as the two magnitudes (3.9) are both large or both small respectively.

Next, in the space group $P\bar{1}$ $\varphi_{\mathbf{k}}$ equals $\varphi_{-\mathbf{k}}$. Hence the result of the preceding paragraph may also be formulated thus: provided the three magnitudes

$$|E_{\mathbf{h}}|,|E_{\mathbf{k}}|,|E_{(\mathbf{h}-\mathbf{k})/2}| \tag{3.11}$$

are all large,

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}\simeq 0 \text{ or } \pi \tag{3.12}$$

according as the two magnitudes

$$|E_{\mathbf{h}-\mathbf{k}}|,|E_{(\mathbf{h}+\mathbf{k})/2}| \tag{3.13}$$

are both large or both small respectively. Therefore the second neighborhood of the structure seminvariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ is defined to be the set of six magnitudes consisting of the four magnitudes (3.5) and the two additional magnitudes

$$|E_{\mathbf{h}\pm\mathbf{k}}|\,. \tag{3.14}$$

The results secured here are summarized schematically by means of Fig. 2 and Table 2.

Table 2. *The probable values of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ in $P\bar{1}$, given the values of five of the six magnitudes in its second neighborhood*

	Magnitudes $\lvert E\rvert$					
φ	**h**	**k**	(**h**+**k**)/2	(**h**−**k**)/2	**h**+**k**	**h**−**k**
0	*L*	*L*	*L*	*L*		*L*
0	*L*	*L*	*L*	*L*	*L*	
π	*L*	*L*	*S*	*L*		*S*
π	*L*	*L*	*L*	*S*	*S*	

Clearly if all six magnitudes in the second neighborhood are large then $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ is expected to be 0 with very high probability. In view of the contradictory entries in the third and fourth rows of Table 2, the estimate π for $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ cannot be made with equally high probability. It is therefore suggested that conditional distributions, given each of the five-magnitude subsets

$$|E_{\mathbf{h}}|,|E_{\mathbf{k}}|,|E_{(\mathbf{h}+\mathbf{k})/2}|,|E_{(\mathbf{h}-\mathbf{k})/2}|,|E_{\mathbf{h}+\mathbf{k}}|\,, \tag{3.15}$$

$$|E_{\mathbf{h}}|,|E_{\mathbf{k}}|,|E_{(\mathbf{h}+\mathbf{k})/2}|,|E_{(\mathbf{h}-\mathbf{k})/2}|,|E_{\mathbf{h}-\mathbf{k}}|\,, \tag{3.16}$$

of the six-magnitude neighborhood, be derived. It is anticipated that the gain in going to the full six magnitude neighborhood will be at best marginal.

IV. The three-phase structure seminvariant, $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$, in $P\bar{1}$

In this space group the linear combination of three phases

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}} \tag{4.1}$$

is a structure seminvariant if and only if

$$\mathbf{h}+\mathbf{k}+\mathbf{l}\equiv 0 \pmod{\boldsymbol{\omega}_s} \tag{4.2}$$

where $\boldsymbol{\omega}_s$, the seminvariant modulus, is defined by (2.3).

IV. 1. *The first neighborhood*

Assume that (4.2) holds so that the components of all four of $(\mathbf{h}\pm\mathbf{k}\pm\mathbf{l})/2$ are integers. Construct the three structure invariants

$$\varphi_{\mathbf{h}}+\varphi_{-(\mathbf{h}+\mathbf{k}-\mathbf{l})/2}+\varphi_{-(\mathbf{h}-\mathbf{k}+\mathbf{l})/2}\,, \tag{4.3}$$

$$\varphi_{\mathbf{k}}+\varphi_{-(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}+\varphi_{-(\mathbf{h}+\mathbf{k}-\mathbf{l})/2}\,, \tag{4.4}$$

$$\varphi_{\mathbf{l}}+\varphi_{-(\mathbf{h}-\mathbf{k}+\mathbf{l})/2}+\varphi_{-(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}\,. \tag{4.5}$$

It is known (4.3) is equal to 0 with high probability provided $|E_{\mathbf{h}}|,|E_{(\mathbf{h}+\mathbf{k}-\mathbf{l})/2}|,|E_{(\mathbf{h}-\mathbf{k}+\mathbf{l})/2}|$ are all large, and similarly with (4.4) and (4.5). Assume then that the six magnitudes

$$|E_{\mathbf{h}}|,|E_{\mathbf{k}}|,|E_{\mathbf{l}}|,|E_{(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}|,|E_{(\mathbf{h}-\mathbf{k}+\mathbf{l})/2}|, +|E_{(\mathbf{h}+\mathbf{k}-\mathbf{l})/2}| \tag{4.6}$$

are all large so that each of (4.3), (4.4), (4.5) is probably equal to 0. Hence (4.3)–(4.5) imply, by addition, $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}=0$ with high probability, *i.e.*

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}\simeq 0\,, \tag{4.7}$$

and the larger the values of the six magnitudes (4.6) the more likely it is that (4.7) holds. However, **h** may be replaced by $-\mathbf{h}$, or **k** by $-\mathbf{k}$, or **l** by $-\mathbf{l}$ without changing the value of the structure seminvariant (4.7).

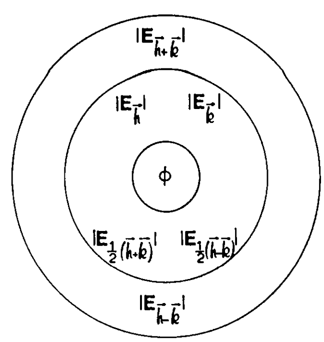

Fig. 2. The first two neighborhoods of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ in $P\bar{1}$.

The first neighborhood of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ is therefore defined to be the set of seven magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{(\mathbf{h}\pm\mathbf{k}\pm\mathbf{l})/2}| \tag{4.8}$$

and the larger the values of these seven magnitudes the more likely it is that (4.7) holds. Since one cannot determine the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ with high probability unless $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|$ are all large, it follows that $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}=\pi$ with high probability only if at least one of the four magnitudes $|E_{(\mathbf{h}\pm\mathbf{k}\pm\mathbf{l})/2}|$ is small. This result is sharpened with the aid of the second neighborhood defined in the next section.

IV. 2. *The second neighborhood*

Construct the two structure invariants

$$\varphi_{\mathbf{h}}+\varphi_{-(\mathbf{h}+\mathbf{k}+\mathbf{l})/2}+\varphi_{(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}\,, \tag{4.9}$$

$$\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{-(\mathbf{h}+\mathbf{k}+\mathbf{l})/2}+\varphi_{-(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}\,. \tag{4.10}$$

Assume first that $|E_{\mathbf{h}}|, |E_{(\mathbf{h}+\mathbf{k}+\mathbf{l})/2}|, |E_{(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}|$ are all large so that the value of (4.9) is probably 0. In order to estimate the value of (4.10) with high probability it is necessary to assume also that $|E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{(\mathbf{h}+\mathbf{k}+\mathbf{l})/2}|, |E_{(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}|$ are all large. Then it is known that the value of (4.10) is probably 0 or π according as $|E_{\mathbf{k}+\mathbf{l}}|, |E_{(\mathbf{h}+\mathbf{k}-\mathbf{l})/2}|, |E_{(\mathbf{h}-\mathbf{k}+\mathbf{l})/2}|$ are all large or all small respectively (Hauptman & Green, 1976). Since every phase in $P\bar{1}$ is 0 or π, addition of (4.9) to (4.10) then yields the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$. In summary then,

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}\simeq 0 \text{ or } \pi \tag{4.11}$$

provided first that the five magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{(\mathbf{h}+\mathbf{k}+\mathbf{l})/2}|, |E_{(-\mathbf{h}+\mathbf{k}+\mathbf{l})/2}| \tag{4.12}$$

are all large, and second that the three magnitudes

$$|E_{\mathbf{k}+\mathbf{l}}|, |E_{(\mathbf{h}-\mathbf{k}+\mathbf{l})/2}|, |E_{(\mathbf{h}+\mathbf{k}-\mathbf{l})/2}| \tag{4.13}$$

are all large or all small respectively. Since $\mathbf{h},\mathbf{k},\mathbf{l}$ may be permuted in any way and $\mathbf{h}$ may be replaced by $-\mathbf{h}$, $\mathbf{k}$ by $-\mathbf{k}$, or $\mathbf{l}$ by $-\mathbf{l}$ without changing the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$, it follows that the second neighborhood of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ is obtained by adjoining to the seven magnitudes of the first neighborhood (4.8) the following six magnitudes:

$$|E_{\mathbf{h}\pm\mathbf{k}}|, |E_{\mathbf{k}\pm\mathbf{l}}|, |E_{\mathbf{l}\pm\mathbf{h}}|\,. \tag{4.14}$$

Furthermore

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}\simeq 0 \text{ or } \pi \tag{4.15}$$

in accordance with the entries of Table 3. In particular, if all or almost all of the 13 magnitudes in the second neighborhood happen to be large then, with near certainty, the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ is 0. Again, the system of neighborhoods for the seminvariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ is shown schematically in Fig. 3.

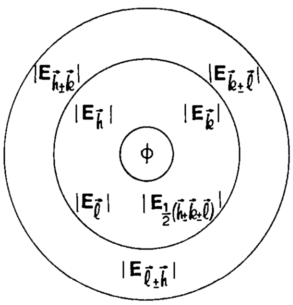

Fig. 3. The first two neighborhoods of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ in $P\bar{1}$.

Table 3. *The probable value of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$ in $P\bar{1}$, given the values of eight of the thirteen magnitudes in its second neighborhood*

		Magnitudes $\lvert E\rvert$												
Row	ϕ	$\vec{h}$	$\vec{k}$	$\vec{\ell}$	$\vec{h}+\vec{k}$	$\vec{k}+\vec{\ell}$	$\vec{\ell}+\vec{h}$	$\vec{h}-\vec{k}$	$\vec{k}-\vec{\ell}$	$\vec{\ell}-\vec{h}$	$\frac{1}{2}(\vec{h}+\vec{k}+\vec{\ell})$	$\frac{1}{2}(-\vec{h}+\vec{k}+\vec{\ell})$	$\frac{1}{2}(\vec{h}-\vec{k}+\vec{\ell})$	$\frac{1}{2}(\vec{h}+\vec{k}-\vec{\ell})$
1	0	L	L	L	L						L	L	L	L
2	0	L	L	L		L					L	L	L	L
3	0	L	L	L			L				L	L	L	L
4	0	L	L	L				L			L	L	L	L
5	0	L	L	L					L		L	L	L	L
6	0	L	L	L						L	L	L	L	L
7	π	L	L	L	S						L	S	S	L
8	π	L	L	L		S					L	L	S	S
9	π	L	L	L			S				L	S	L	S
10	π	L	L	L				S			S	L	L	S
11	π	L	L	L					S		S	S	L	L
12	π	L	L	L						S	S	L	S	L

Since no two of the rows 7–12 of Table 3 are mutually reinforcing, the derivation of the conditional probability distribution of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}$, given all 13 magnitudes of the second neighborhood, is not recommended. It is suggested instead that the distribution, given all seven magnitudes of the first neighborhood, be found first. It would then be instructive to derive the six distributions, given the eight magnitude subsets of the complete second neighborhood shown in rows 7–12 of Table 3.

V. The four-phase structure seminvariant, $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, in $P\bar{1}$

Once again, the linear combination of four phases

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \tag{5.1}$$

is a structure seminvariant if and only if

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}\equiv 0 \pmod{\boldsymbol{\omega}_s} \tag{5.2}$$

where $\boldsymbol{\omega}_s$ is defined by (2.3).

V. 1. *The first neighborhood*

Proceeding as in §§3.1 and 4.1 one is led to define the first neighborhood of the structure seminvariant (5.1) as consisting of the set of 12 magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}| , \tag{5.3}$$

$$|E_{(\mathbf{h}\pm\mathbf{k}\pm\mathbf{l}\pm\mathbf{m})/2}| , \tag{5.4}$$

and to infer that if most or all of the 12 magnitudes (5.3) and (5.4) are large then (5.1) is probably equal to 0.

V. 2. *The second neighborhood*

Construct the two structure invariants

$$\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{-(\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m})/2} + \varphi_{-(\mathbf{h}+\mathbf{k}-\mathbf{l}-\mathbf{m})/2} , \tag{5.5}$$

$$\varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} + {}_{-(\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m})/2} + \varphi_{(\mathbf{h}+\mathbf{k}-\mathbf{l}-\mathbf{m})/2} . \tag{5.6}$$

In order to estimate the values of (5.5) and (5.6) with high probability it is necessary to assume first that all six magnitudes

$$|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{(\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m})/2}|, |E_{(\mathbf{h}+\mathbf{k}-\mathbf{l}-\mathbf{m})/2}| \tag{5.7}$$

are large. Then (5.5) is probably 0 or π according as the three magnitudes

$$|E_{\mathbf{h}+\mathbf{k}}|, |E_{(\mathbf{h}-\mathbf{k}+\mathbf{l}+\mathbf{m})/2}|, |E_{(-\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m})/2}|$$

are all large or all small respectively (Hauptman & Green, 1976). Again, (5.6) is probably 0 or π according as the three magnitudes

$$|E_{\mathbf{l}+\mathbf{m}}|, |E_{(\mathbf{h}+\mathbf{k}+\mathbf{l}-\mathbf{m})/2}|, |E_{(\mathbf{h}+\mathbf{k}-\mathbf{l}+\mathbf{m})/2}|$$

are all large or all small respectively. Since every phase equals 0 or π, addition of (5.5) to (5.6) yields the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$. In summary then,

$$\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}} \simeq 0 \tag{5.8}$$

provided first that the six magnitudes (5.7) are all large, and second that the six magnitudes

$$|E_{\mathbf{h}+\mathbf{k}}|, |E_{(-\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m})/2}|, |E_{(\mathbf{h}-\mathbf{k}+\mathbf{l}+\mathbf{m})/2}| , \tag{5.9}$$

$$|E_{\mathbf{l}+\mathbf{m}}|, |E_{(\mathbf{h}+\mathbf{k}-\mathbf{l}+\mathbf{m})/2}|, |E_{(\mathbf{h}+\mathbf{k}+\mathbf{l}-\mathbf{m})/2}| \tag{5.10}$$

are all large or all small. If, on the other hand, all six

Table 4. *The probable value of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in $P\bar{1}$, given the values of* 12 *of the* 24 *magnitudes in its second neighborhood*

The entries refer to the values of $|E|$.

		Magnitudes $\|E\|$																											
Row	ϕ	$\vec{h}$	$\vec{k}$	$\vec{\ell}$	$\vec{m}$	$\vec{h}+\vec{k}$	$\vec{\ell}+\vec{m}$	$\vec{h}+\vec{\ell}$	$\vec{k}+\vec{m}$	$\vec{h}+\vec{m}$	$\vec{k}+\vec{\ell}$	$\vec{h}-\vec{k}$	$\vec{\ell}-\vec{m}$	$\vec{h}-\vec{\ell}$	$\vec{k}-\vec{m}$	$\vec{h}-\vec{m}$	$\vec{k}-\vec{\ell}$	$\frac{1}{2}(\vec{h}+\vec{k}+\vec{\ell}+\vec{m})$	$\frac{1}{2}(\vec{h}+\vec{k}-\vec{\ell}-\vec{m})$	$\frac{1}{2}(\vec{h}-\vec{k}+\vec{\ell}-\vec{m})$	$\frac{1}{2}(\vec{h}-\vec{k}-\vec{\ell}+\vec{m})$	$\frac{1}{2}(\vec{h}+\vec{k}+\vec{\ell}-\vec{m})$	$\frac{1}{2}(\vec{h}+\vec{k}-\vec{\ell}+\vec{m})$	$\frac{1}{2}(\vec{h}-\vec{k}+\vec{\ell}+\vec{m})$	$\frac{1}{2}(-\vec{h}+\vec{k}+\vec{\ell}+\vec{m})$
1	0	L	L	L	L	L	L											L	L			L	L	L	L
2	0	L	L	L	L			L	L									L		L		L	L	L	L
3	0	L	L	L	L					L	L							L			L	L	L	L	L
4	0	L	L	L	L							L	L							L	L	L	L	L	L
5	0	L	L	L	L									L	L				L		L	L	L	L	L
6	0	L	L	L	L											L	L		L	L		L	L	L	L
7	0	L	L	L	L	L							L					L	L	L	L	L	L		
8	0	L	L	L	L		L					L						L	L	L	L			L	L
9	0	L	L	L	L			L							L			L	L	L	L	L		L	
10	0	L	L	L	L				L					L				L	L	L	L		L		L
11	0	L	L	L	L					L							L	L	L	L	L		L	L	
12	0	L	L	L	L						L					L		L	L	L	L	L			L
13	0	L	L	L	L	S	S											L	L			S	S	S	S
14	0	L	L	L	L			S	S									L		L		S	S	S	S
15	0	L	L	L	L					S	S							L			L	S	S	S	S
16	0	L	L	L	L							S	S							L	L	S	S	S	S
17	0	L	L	L	L									S	S				L		L	S	S	S	S
18	0	L	L	L	L											S	S		L	L		S	S	S	S
19	0	L	L	L	L	S							S					S	S	S	S	L	L		
20	0	L	L	L	L		S					S						S	S	S	S			L	L
21	0	L	L	L	L			S							S			S	S	S	S	L		L	
22	0	L	L	L	L				S					S				S	S	S	S		L		L
23	0	L	L	L	L					S							S	S	S	S	S		L	L	
24	0	L	L	L	L						S					S		S	S	S	S	L			L
25	π	L	L	L	L	L	S											L	L			S	S	L	L
26	π	L	L	L	L			L	S									L		L		S	L	S	L
27	π	L	L	L	L					L	S							L			L	L	S	S	L
28	π	L	L	L	L							L	S							L	L	L	L	S	S
29	π	L	L	L	L									L	S				L		L	L	S	L	S
30	π	L	L	L	L											L	S		L	L		S	L	L	S
31	π	L	L	L	L	L							S					S	S	L	L	L	L		
32	π	L	L	L	L		S					L						L	L	S	S			L	L
33	π	L	L	L	L			L							S			S	L	S	L	L		L	
34	π	L	L	L	L				S					L				L	S	L	S		L		L
35	π	L	L	L	L					L							S	S	L	L	S		L	L	
36	π	L	L	L	L						S					L		L	S	S	L	L			L
37	π	L	L	L	L	S	L											L	L			L	L	S	S
38	π	L	L	L	L			S	L									L		L		L	S	L	S
39	π	L	L	L	L					S	L							L			L	S	L	L	S
40	π	L	L	L	L							S	L							L	L	S	S	L	L
41	π	L	L	L	L									S	L				L		L	S	L	S	L
42	π	L	L	L	L											S	L		L	L		L	S	S	L
43	π	L	L	L	L	S							L					L	L	S	S	L	L		
44	π	L	L	L	L		L					S						S	S	L	L			L	L
45	π	L	L	L	L			S							L			L	S	L	S	L		L	
46	π	L	L	L	L				L					S				S	L	S	L		L		L
47	π	L	L	L	L					S							L	L	S	S	L		L	L	
48	π	L	L	L	L						L					S		S	L	L	S	L			L

magnitudes of (5.7) are large and the three magnitudes in one of the two sets of magnitudes (5.9), (5.10) are all large and in the other all small, then

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}\simeq\pi\,. \tag{5.11}$$

Since $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$ may be permuted in any way and $\mathbf{h}$ may be replaced by $-\mathbf{h}$, $\mathbf{k}$ by $-\mathbf{k}$, $\mathbf{l}$ by $-\mathbf{l}$, or $\mathbf{m}$ by $-\mathbf{m}$ without changing the value of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, it follows that the second neighborhood of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ is obtained by adjoining to the 12 magnitudes of the first neighborhood, (5.3) and (5.4), the following 12 magnitudes:

$$|E_{\mathbf{h}\pm\mathbf{k}}|,|E_{\mathbf{l}\pm\mathbf{m}}|,|E_{\mathbf{h}\pm\mathbf{l}}|,|E_{\mathbf{k}\pm\mathbf{m}}|,|E_{\mathbf{h}\pm\mathbf{m}}|,|E_{\mathbf{k}\pm\mathbf{l}}|\,. \tag{5.12}$$

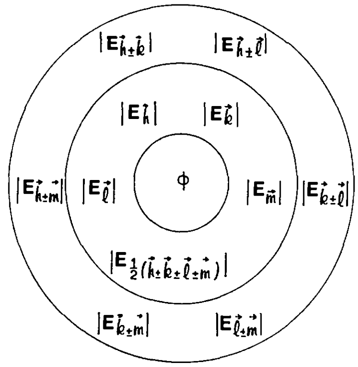

Fig. 4. The first two neighborhoods of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in $P\bar{1}$.

Furthermore

$$\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}\simeq 0 \text{ or } \pi \tag{5.13}$$

in accordance with the entries of Table 4.

Certain of the rows of Table 4 are completely reinforcing. Thus, rows 1–12 are in perfect accord and complementary and are combined to form the first row of Table 5. Similarly, rows 13–18 of Table 4 are in complete agreement and reinforcing and together form the second row of Table 5. Again rows 19–24 of Table 4 combine to give row 3 of Table 5. Next, row 4 of Table 5 is derived from rows 25 and 32 of Table 4 which are in perfect agreement and reinforcing, row 5 of Table 5 from rows 26 and 34 of Table 4, *etc.*

Finally, as before, the first two neighborhoods of the structure seminvariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ are shown schematically in Fig. 4.

In accordance with the entries of Table 5, it is suggested that the conditional probability distribution of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, given the 12 magnitudes in its first neighborhood, be derived first. Three other distributions should then be found by adjoining to the 12 magnitudes of the first neighborhood each of the three sets of four magnitudes

$$|E_{\mathbf{h}\pm\mathbf{k}}|,|E_{\mathbf{l}\pm\mathbf{m}}|\,, \tag{5.14}$$

$$|E_{\mathbf{h}\pm\mathbf{l}}|,|E_{\mathbf{k}\pm\mathbf{m}}|\,, \tag{5.15}$$

$$|E_{\mathbf{h}\pm\mathbf{m}}|,|E_{\mathbf{k}\pm\mathbf{l}}|\,, \tag{5.16}$$

in turn. Owing to the construction of Table 5, by combining reinforcing rows of Table 4, it is anticipated

Table 5. *The probable value of the structure seminvariant* $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ *in* $P\bar{1}$, *given the values of* 15 *or of* 16 *or of all* 24 *of the* 24 *magnitudes in its second neighborhood*; *obtained from Table* 4 *by combining reinforcing rows*

The entries refer to the values of $|E|$.

Magnitudes $|E|$

Rows from Table 4	ϕ	$\vec h$	$\vec k$	$\vec l$	$\vec m$	$\vec h+\vec k$	$\vec l+\vec m$	$\vec h+\vec l$	$\vec k+\vec m$	$\vec h+\vec m$	$\vec k+\vec l$	$\vec h-\vec k$	$\vec l-\vec m$	$\vec h-\vec l$	$\vec k-\vec m$	$\vec h-\vec m$	$\vec k-\vec l$	$\frac{1}{2}(\vec h+\vec k+\vec l+\vec m)$	$\frac{1}{2}(\vec h+\vec k-\vec l-\vec m)$	$\frac{1}{2}(\vec h-\vec k+\vec l-\vec m)$	$\frac{1}{2}(\vec h-\vec k-\vec l+\vec m)$	$\frac{1}{2}(\vec h+\vec k+\vec l-\vec m)$	$\frac{1}{2}(\vec h+\vec k-\vec l+\vec m)$	$\frac{1}{2}(\vec h-\vec k+\vec l+\vec m)$	$\frac{1}{2}(-\vec h+\vec k+\vec l+\vec m)$
1–12	0	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L	L
13–18	0	L	L	L	L	S	S	S	S	S	S	S	S	S	S	S	S	L	L	L	L	S	S	S	S
19–24	0	L	L	L	L	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	L	L	L	L
25,32	π	L	L	L	L	L	S					L						L	L	S	S	S	S	L	L
26,34	π	L	L	L	L			L	S					L				L	S	L	S	S	L	S	L
27,36	π	L	L	L	L					L	S					L		L	S	S	L	L	S	S	L
28,31	π	L	L	L	L	L						L	S					S	S	L	L	L	L	S	S
29,33	π	L	L	L	L			L						L	S			S	L	S	L	L	S	L	S
30,35	π	L	L	L	L					L						L	S	S	L	L	S	S	L	L	S
37,43	π	L	L	L	L	S	L						L					L	L	S	S	L	L	S	S
38,45	π	L	L	L	L			S	L						L			L	S	L	S	L	S	L	S
39,47	π	L	L	L	L					S	L						L	L	S	S	L	S	L	L	S
40,44	π	L	L	L	L		L					S	L					S	S	L	L	S	S	L	L
41,46	π	L	L	L	L				L					S	L			S	L	S	L	S	L	S	L
42,48	π	L	L	L	L						L					S	L	S	L	L	S	L	S	S	L
25,40	π	L	L	L	L	L	S					S	L					L	L	L	L	S	S	L	L
26,41	π	L	L	L	L			L	S					S	L			L	L	L	L	S	L	S	L
27,42	π	L	L	L	L					L	S					S	L	L	L	L	L	L	S	S	L
28,37	π	L	L	L	L	S	L					L	S					L	L	L	L	L	L	S	S
29,38	π	L	L	L	L			S	L					L	S			L	L	L	L	L	S	L	S
30,39	π	L	L	L	L					S	L					L	S	L	L	L	L	S	L	L	S
31,44	π	L	L	L	L	L	L					S	S					S	S	L	L	L	L	L	L
32,43	π	L	L	L	L	S	S					L	L					L	L	S	S	L	L	L	L
33,46	π	L	L	L	L			L	L					S	S			S	L	S	L	L	L	L	L
34,45	π	L	L	L	L			S	S					L	L			L	S	L	S	L	L	L	L
35,48	π	L	L	L	L					L	L					S	S	S	L	L	S	L	L	L	L
36,47	π	L	L	L	L					S	S					L	L	L	S	S	L	L	L	L	L

that these distributions will have the potential to yield reliable estimates for the four-phase structure seminvariants $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, *i.e.* that many of the distributions will have a very small variance. However, comparison of the different rows of Table 5 reveals significant contradictions. It is therefore not recommended that the conditional probability distribution of $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, given all 24 magnitudes in its second neighborhood, be derived. Although the 24-magnitude estimate may be somewhat superior to the 12 or the three 16-magnitude estimates, it is anticipated that the improvement will be at best marginal and hardly worth the additional effort to derive or the time to calculate.

VI. Concluding remarks

The first two neighborhoods of each of the structure seminvariants, $\varphi_{\mathbf{h}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}, \varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, in the space group $P\bar{1}$ have been found. In this way those magnitudes are identified on which the value of the structure seminvariant chiefly depends, and the qualitative relation between the seminvariant and the magnitudes in the appropriate neighborhood (or subset) is derived. The task of determining the more precise relation, *i.e.* the conditional probability distribution of the structure seminvariant, given the magnitudes in the neighborhood, or an appropriate subset, remains to be completed. For the structure seminvariants $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ this task has been done for the first neighborhood and is described in the accompanying paper (Green & Hauptman, 1976). In view of this work it is anticipated that the remaining task, though time consuming, will not present insurmountable obstacles.

Next, there remains the problem of identifying the neighborhoods of the structure seminvariants in other space groups, in particular $P2_1$ and $P2_12_12_1$. It is anticipated that the methods described here will carry over to these space groups without essential change. Once this is done the derivation of the appropriate probability distributions in these space groups is called for. In view of our limited experience, it seems impossible to evaluate now the magnitude or difficulty of this task or the extent to which present methods, successful in the space groups $P1$ and $P\bar{1}$, will be applicable to the remaining space groups. However, some preliminary work along these lines suggests that the task will not present insuperable difficulties.

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A Conditional Probability Distribution of the Structure Seminvariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$ in $P\bar{1}$: Effects of Higher-Order Terms

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A crystal structure in $P\bar{1}$ consisting of N identical atoms in the whole unit cell is fixed, and the four non-negative numbers $R_1, R_2, R_{12/2}, R_{1\bar{2}/2}$ are also specified. The random variables (vectors) $\mathbf{h},\mathbf{k}$ are assumed to be uniformly and independently distributed in the regions of reciprocal space defined by $|E_{\mathbf{h}}|=R_1, |E_{\mathbf{k}}|=R_2, |E_{(\mathbf{h}+\mathbf{k})/2}|=R_{12/2}, |E_{(\mathbf{h}-\mathbf{k}/2)}|=R_{1\bar{2}/2}$, (1), and $\mathbf{h}+\mathbf{k}\equiv 0 \pmod{\boldsymbol{\omega}_s}$, (2), where $\boldsymbol{\omega}_s$, the seminvariant modulus for $P\bar{1}$, is the three-dimensional vector $\boldsymbol{\omega}_s=(2,2,2)$, (3). Then the components of each of $(\mathbf{h}\pm\mathbf{k})/2$ are integers. In view of (2) and (3) the linear combination of the phases $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}$, (4), is a structure seminvariant which, as a function of the primitive random variables $\mathbf{h},\mathbf{k}$, is itself a random variable. Two approximations $Q_{\pm}, P_{\pm}$, of respective orders $1/N$, $1/N^2$, to the conditional probability distribution of φ, given the four magnitudes (1), are derived and compared. In favorable cases, *i.e.* when the variance of the distribution happens to be small, they yield a reliable estimate (0 or π) for the structure seminvariant φ.

I. Introduction

Recently secured methods in the probabilistic theory of the structure invariants (Hauptman, 1975*a*,*b*; Green & Hauptman, 1976; Hauptman & Green, 1976) are applied here to the determination of the conditional distribution of the two-phase structure seminvariant

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}} \tag{1.1}$$