Acta Cryst. (1978). A**34**, 27–30

The Estimation in $P\bar{1}$ of Two-Phase and Three-Phase Structure Seminvariants *via* their First Representations

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(*Received* 25 *May* 1977; *accepted* 19 *June* 1977)

A probabilistic theory is described which is able to estimate in $P\bar{1}$ the values of two and three-phase structure seminvariants. In particular, up to six and seventeen moduli may be exploited in order to estimate two and three-phase seminvariants respectively.

1. Introduction

Probabilistic theories of the two-phase seminvariants in $P\bar{1}$ have been described by Giacovazzo (1974) and by Green & Hauptman (1976). Both theories are able to estimate the value of $S(\mathbf{h}_1 + \mathbf{h}_2)S(\mathbf{h}_1 - \mathbf{h}_2)$ by the joint probability distribution

$$P(E_{\mathbf{h}_1}, E_{\mathbf{h}_2}, E_{\mathbf{h}_1+\mathbf{h}_2}, E_{\mathbf{h}_1-\mathbf{h}_2}). \qquad (1)$$

A common result is that relations of the type

$$S(\mathbf{h}_1 + \mathbf{h}_2)S(\mathbf{h}_1 - \mathbf{h}_2) = -1$$

arise when the $|E|$'s involved in (1) have suitable values. (1) involves the same structure factors which appear in the system

$$S(\mathbf{h}_1)S(\mathbf{h}_2) \simeq S(\mathbf{h}_1 + \mathbf{h}_2),$$

$$S(\mathbf{h}_1)S(\mathbf{h}_2) \simeq S(\mathbf{h}_1 - \mathbf{h}_2).$$

When all the $|E|$'s are large the system gives $S(\mathbf{h}_1 + \mathbf{h}_2) \simeq S(\mathbf{h}_1 - \mathbf{h}_2)$. Therefore we say that the study of (1) leads in $P\bar{1}$ to the probabilistic theories of the coincidence method (Grant, Howells & Rogers, 1957). A probabilistic theory of the coincidence method valid in all the space groups has recently been described by Giacovazzo (1977*a*,*b*).

The theory of representations (Giacovazzo, 1977*c*) has given the author new insights into probabilistic methods of obtaining accurate estimates of the phase invariants and seminvariants. This theory is able, for any universal structure invariant or structure seminvariant Φ, to arrange in a general way the set of reflexions in a sequence of subsets, each contained in the succeeding one, whose order is that of the expected effectiveness (in the statistical sense) for the estimation of Φ. From each subset $\{B\}_n$, which was called the phasing shell of nth order for Φ, one is able to estimate a collection of structure invariants (denoted in the quoted paper as $\{\Psi\}_n$) whose values may differ from Φ by constants which arise because of translational symmetry. In $P\bar{1}$ the first representation of the two-phase seminvariants $\Phi = \varphi_{\mathbf{h}_1+\mathbf{h}_2} + \varphi_{\mathbf{h}_1-\mathbf{h}_2}$ is shown to be the collection of the two quartet invariants

$$\Psi'_1 = \varphi_{\mathbf{h}_1+\mathbf{h}_2} + \varphi_{\mathbf{h}_1-\mathbf{h}_2} - \varphi_{\mathbf{h}_1} - \varphi_{\mathbf{h}_1},$$

$$\Psi''_1 = \varphi_{\mathbf{h}_1+\mathbf{h}_2} - \varphi_{\mathbf{h}_1-\mathbf{h}_2} - \varphi_{\mathbf{h}_2} - \varphi_{\mathbf{h}_2}.$$

The first phasing shell of Φ (*i.e.* the collection of the basis and of the cross-magnitudes of the quartet invariants) is then

$$\{B\}_1 = \{|E_{\mathbf{h}_1}|, |E_{\mathbf{h}_2}|, |E_{\mathbf{h}_1+\mathbf{h}_2}|, |E_{\mathbf{h}_1-\mathbf{h}_2}|, |E_{2\mathbf{h}_1}|, |E_{2\mathbf{h}_2}|\}.$$

In conclusion, the theory of representations lets us know that Φ depends in the first instance on six magnitudes, two of which (*i.e.* $|E_{2\mathbf{h}_1}|$ and $|E_{2\mathbf{h}_2}|$) were not considered in the coincidence method.

The first aim of this paper is to estimate in $P\bar{1}$ the two-phase seminvariants by means of their first representation. Thus in § 2 the joint distribution

$$P(E_{\mathbf{h}_1}, E_{\mathbf{h}_2}, E_{\mathbf{h}_1+\mathbf{h}_2}, E_{\mathbf{h}_1-\mathbf{h}_2}, E_{2\mathbf{h}_1}, E_{2\mathbf{h}_2}) \qquad (2)$$

will be studied. The second aim of this paper is to estimate in $P\bar{1}$ the three-phase structure seminvariants [*i.e.* $\Phi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}}$ where $\mathbf{h} + \mathbf{k} + \mathbf{l} \equiv 0$ mod(222)] by means of their first representation. In accordance with Giacovazzo (1977*c*) the first representation of $\Phi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{h}+\mathbf{k}+2\mathbf{l}}$ is the collection of the quintet invariants:

$$\Psi'_1 = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + 2\varphi_{\mathbf{l}} - \varphi_{\mathbf{h}+\mathbf{k}+2\mathbf{l}},$$

$$\Psi''_1 = -\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} = 2\varphi_{\mathbf{h}+\mathbf{l}} - \varphi_{\mathbf{h}+\mathbf{k}+2\mathbf{l}},$$

$$\Psi'''_1 = \varphi_{\mathbf{h}} - \varphi_{\mathbf{k}} + 2\varphi_{\mathbf{k}+\mathbf{l}} - \varphi_{\mathbf{h}+\mathbf{k}+2\mathbf{l}},$$

$$\Psi''''_1 = \varphi_{\mathbf{h}} - \varphi_{\mathbf{k}} + 2\varphi_{\mathbf{h}+\mathbf{k}+\mathbf{l}} - \varphi_{\mathbf{h}+\mathbf{k}+2\mathbf{l}}.$$

The first phasing shell of Φ (*i.e.* the collection of the basis and of the cross-magnitudes of the quintet invariants) is then

$$\{B\}_1 = \{|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{h}+\mathbf{k}+2\mathbf{l}}|, |E_{\mathbf{l}}|, |E_{\mathbf{h}+\mathbf{l}}|, |E_{\mathbf{k}+\mathbf{l}}|, |E_{\mathbf{h}+\mathbf{k}+\mathbf{l}}|, |E_{\mathbf{h}+\mathbf{k}}|, |E_{\mathbf{h}-\mathbf{k}}|, |E_{\mathbf{h}+2\mathbf{l}}|, |E_{\mathbf{k}+2\mathbf{l}}|, |E_{\mathbf{h}+2\mathbf{k}+2\mathbf{l}}|, |E_{2\mathbf{h}+\mathbf{k}+2\mathbf{l}}|, |E_{2\mathbf{l}}|, |E_{2\mathbf{h}+2\mathbf{l}}|, |E_{2\mathbf{k}+2\mathbf{l}}|, |E_{2\mathbf{h}+2\mathbf{k}+2\mathbf{l}}|\}.$$

The joint probability distribution of the above 17 structure factors will be studied in § 3.

In our probabilistic approach we will assume the reciprocal vectors are fixed and the atomic coordinates are the primitive random variables. Two different mathematical methods will be used. The first involves a Gram–Charlier expansion of the characteristic function; the second directly uses the exponential form of the characteristic function. Only conclusive formulae will be given here. The reader will find a general account of the methods in Giacovazzo (1976) for the estimation of the quartet invariants which are elements of the first representation of the two-phase seminvariants, in Giacovazzo (1977*d*) for the estimation of the quintets which are elements of the first representation of the three-phase structure seminvariants.

2. The estimation of $\varphi_{\mathbf{h}_1+\mathbf{h}_2} + \varphi_{\mathbf{h}_1-\mathbf{h}_2}$ in $P\bar{1}$ via its first representation

In accordance with § 1 we have studied the joint probability distribution function (2). We denote by $E_1, E_2, \ldots, E_6$ the normalized structure factors $E_{\mathbf{h}_1}, E_{\mathbf{h}_2}, \ldots, |E_{2\mathbf{h}_2}|$ respectively, by R_i, $i = 1, \ldots, 6$ their moduli, and by P_+ the probability that E_3E_4 is positive. Using the Gram–Charlier expansion of the characteristic function we obtain

$$P_+ = 0{\cdot}5 + 0{\cdot}5 \tanh\left(\frac{R_3R_4}{2N}\frac{A}{B}\right), \tag{3}$$

where

$$A = \varepsilon_1 + \varepsilon_2 + \varepsilon_1\varepsilon_5 + 2\varepsilon_1\varepsilon_2 + \varepsilon_2\varepsilon_6,$$

$$B = 1 - \sum_{i=1}^{6} H_4(E_i)/8N + (\varepsilon_1\varepsilon_2\varepsilon_3 + \varepsilon_1\varepsilon_2\varepsilon_4 + \varepsilon_3\varepsilon_4\varepsilon_5 + \varepsilon_3\varepsilon_4\varepsilon_6)/2N,$$

$$\varepsilon_i = (E_i^2 - 1).$$

$H_4(x)$ is the Hermite polynomial of order four defined by

$$H_4(x) = x^4 - 6x^2 + 3.$$

The number of two-phase seminvariants for which all the six reflexions in (2) are in the set of measured reflexions may be a small percentage of the observable two-phase seminvariants. Thus it might be useful to use marginal probability densities of (2). In these cases the probability values can be easily derived from (3) by making equal to zero the terms ε_i corresponding to the magnitudes R_i which are not in the measurements. In particular, if both R_5 and R_6 are not in the measurements, (3) reduces to

$$P_+ \simeq 0{\cdot}5 + 0{\cdot}5 \tanh\left(\frac{R_3R_4}{2N}\cdot\frac{A'}{B'}\right), \tag{4}$$

where

$$A' = \varepsilon_1 + \varepsilon_2 + 2\varepsilon_1\varepsilon_2$$

$$B' = 1 - \sum_{i=1}^{4} H_4(E_i)/8N + [\varepsilon_1\varepsilon_2\varepsilon_3 + \varepsilon_1\varepsilon_2\varepsilon_4]/2N,$$

(4) practically coincides with (11) in Giacovazzo's (1974) paper.

If the Fourier transform of the exponential form of the characteristic function is directly used, the probability that E_3E_4 is positive is given by

$$P_+ = \frac{P_+^0}{P_+^0 + P^0}, \tag{5}$$

where

$$\begin{aligned} P_\pm^0 = {} & \exp(\mp B) \\ & \times [\exp(+A_6^\pm \pm A_{1,2}^\pm \mp A_{1,2,6}^\pm)\cosh(A_5^\pm - A_{5,6} \mp A_{1,2,5}^\pm) \\ & + \exp(-A_6^\pm \pm A_{1,2}^\pm \pm A_{1,2,6}^\pm)\cosh(A_5^\pm + A_{5,6} \mp A_{1,2,5}^\pm) \\ & + \exp(+A_6^\pm \mp A_{1,2}^\pm \pm A_{1,2,6}^\pm)\cosh(A_5^\pm - A_{5,6} \pm A_{1,2,5}^\pm) \\ & + \exp(-A_6^\pm \mp A_{1,2}^\pm \mp A_{1,2,6}^\pm)\cosh(A_5^\pm + A_{5,6} \pm A_{1,2,5}^\pm)], \end{aligned} \tag{6}$$

where

$$B = (R_1^2 + R_2^2)R_3R_4/N,$$

$$A_5^\pm = \left(\frac{R_1^2}{2} \pm R_3R_4\right)R_5/\sqrt{N},$$

$$A_6^\pm = \left(\frac{R_2^2}{2} \pm R_3R_4\right)R_6/\sqrt{N},$$

$$A_{1,2}^\pm = R_1R_2(R_3 \pm R_4)/\sqrt{N},$$

$$A_{5,6} = R_5R_6(R_3^2 + R_4^2)/2N,$$

$$A_{1,2,5}^\pm = R_1R_2R_5(R_3 \pm R_4)/N,$$

$$A_{1,2,6}^\pm = R_1R_2R_6(R_3 \pm R_4)/N.$$

The sign probabilities from marginal distributions may be easily derived from (5) by making equal to zero in (6) the R's corresponding to the non-observed reflexions and by replacing B by the following expression:

$$B = \mathrm{IND1}\left(\frac{R_1^2R_3R_4}{N}\right) + \mathrm{IND2}\left(\frac{R_2^2R_3R_4}{N}\right), \tag{7}$$

where: IND1 = 1; 0·5 according to whether R_5 is in the measurements or not; IND2 = 1; 0·5 according to whether R_6 is in the measurements or not.

In (6) the terms $A_{1,2,6}$, $A_{5,6}$, $A_{1,2,5}$ are of order $1/N$. If they are neglected in comparison with $A_6 \pm A_{1,2}$ and with A_5, (6) reduces to

$$P_\pm^0 = \exp(\mp B)\cosh A_5^\pm \cosh A_6^\pm \cosh A_{1,2}^\pm. \tag{8}$$

Of course, if R_5 or R_6 are not in the measurements,

B varies according to (7). In particular if R_5 and R_6 are unknown, (7) and (8) reduce to

$$P_{\pm}^{0} = \exp(\mp B)\cosh A_{1,2}^{\pm} \qquad (9)$$

which coincides with (4.10) of Green & Hauptman (1976) or with (20) of Giacovazzo (1977*a*) when (20) is calculated in $P\bar{1}$.

3. Calculations

A model structure in $P\bar{1}$ consisting of $N = 40$ identical atoms in the unit cell was constructed. With the 118 $|E|$'s greater than 1·6 (*i.e.* $|E_{\mathbf{h}_1+\mathbf{h}_2}| > 1{\cdot}6$, $|E_{\mathbf{h}_1-\mathbf{h}_2}| > 1{\cdot}6$), 167 two-phase seminvariants were calculated according to (3), (4), (6), (8), (9) and the first 30 of these arranged in descending order of the expected accuracy provided by (3) (Table 1). The contribution of the Hermite polynomials of order four in (3) and (4) proved negligible. In order to save computing time we have excluded them from our calculations. The column headed cos(T) in Table 1 lists the true values of $\cos(\varphi_{\mathbf{h}_1+\mathbf{h}_2} + \varphi_{\mathbf{h}_1-\mathbf{h}_2})$. Inspection of Table 1 shows: (*a*) all the seminvariants are correctly estimated by (3); (*b*) (4) and (9) seem to be equivalent in many cases; (*c*) (4) and (9) wrongly estimate seminvariants No. 17 and 30, on the other hand (3), (6) and (8) provide their correct signs; (*d*) (6) wrongly estimates seminvariants No. 12, 18, 21 which are well estimated by (3). Furthermore (8) correctly estimates 12 and 21.

These considerations lead to the use of (3) and (8) in the direct procedures for phase solution.

4. The estimation of the three-phase seminvariants in $P\bar{1}$ *via* its first representation

Let $\Phi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{h}+\mathbf{k}+2\mathbf{l}}$ be our seminvariant. In accordance with § 1 we have studied the joint probability distribution function

$$P(E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{h}+\mathbf{k}+2\mathbf{l}}, E_{\mathbf{l}}, E_{\mathbf{h}+\mathbf{l}}, E_{\mathbf{k}+\mathbf{l}}, E_{\mathbf{h}+\mathbf{k}+\mathbf{l}}, E_{\mathbf{h}+\mathbf{k}}, E_{\mathbf{h}-\mathbf{k}}, E_{\mathbf{h}+2\mathbf{l}}, E_{\mathbf{k}+2\mathbf{l}}, E_{\mathbf{h}+2\mathbf{k}+2\mathbf{l}}, E_{2\mathbf{h}+\mathbf{k}+2\mathbf{l}}, E_{2\mathbf{l}}, E_{2\mathbf{h}+2\mathbf{l}}, E_{2\mathbf{k}+2\mathbf{l}}, E_{2\mathbf{h}+2\mathbf{k}+2\mathbf{l}}).$$

We denote by $E_1, E_2, \ldots, E_{17}$ the normalized structure factors $E_{\mathbf{h}}, E_{\mathbf{k}}, \ldots, E_{2\mathbf{h}+2\mathbf{k}+2\mathbf{l}}$, respectively, by R_i, $i = 1, \ldots, 17$ their moduli and by P_+ the probability that

Table 1. 30 *values of sign probabilities for two-phase seminvariants as given by* (3), (6), (8), (4), (9) *for a model structure in* $P\bar{1}$ *with* $N = 40$ *atoms in the unit cell*

The asterisk denotes the magnitudes which are not in the measurements.

No.	$E_{\mathbf{h}_1}$	$E_{\mathbf{h}_2}$	$E_{\mathbf{h}_1+\mathbf{h}_2}$	$E_{\mathbf{h}_1-\mathbf{h}_2}$	$E_{2\mathbf{h}_1}$	$E_{2\mathbf{h}_2}$	cos(T)	(3)	(6)	(8)	(4)	(9)
1	1·05	3·45	2·10	2·22	0·37	1·80	1·0	0·96	0·58	0·74	0·80	0·57
2	2·76	2·48	1·61	1·98	2·24	*	1·0	0·94	0·87	0·96	0·90	0·88
3	3·45	2·13	2·24	2·48	1·80	1·33	1·0	0·93	0·72	0·97	0·91	0·92
4	2·76	1·91	1·77	1·77	2·24	*	1·0	0·93	0·82	0·93	0·86	0·80
5	2·76	1·80	1·92	1·99	2·24	0·16	1·0	0·93	0·78	0·91	0·86	0·79
6	3·45	2·08	1·65	2·64	1·80	*	1·0	0·93	0·81	0·94	0·89	0·87
7	2·76	1·82	1·87	2·28	2·24	*	1·0	0·93	0·83	0·94	0·86	0·80
8	2·76	2·28	1·82	2·52	2·24	*	1·0	0·92	0·85	0·96	0·89	0·87
9	2·76	2·28	1·81	2·52	2·24	*	1·0	0·92	0·85	0·96	0·88	0·87
10	1·98	2·76	1·80	2·48	*	2·24	1·0	0·92	0·83	0·95	0·87	0·83
11	1·56	2·76	2·24	2·30	*	2·24	1·0	0·92	0·81	0·92	0·85	0·75
12	3·45	1·76	1·98	2·76	1·80	2·48	1·0	0·91	0·41	0·96	0·90	0·82
13	2·76	1·77	1·91	3·03	2·24	*	1·0	0·91	0·75	0·93	0·86	0·77
14	3·03	3·45	2·05	3·32	*	1·80	1·0	0·91	0·79	0·98	0·89	0·96
15	1·10	2·76	1·62	2·13	*	2·24	1·0	0·91	0·73	0·83	0·68	0·59
16	1·34	2·76	1·89	3·32	*	2·24	1·0	0·90	0·66	0·87	0·82	0·64
17	2·76	0·01	2·08	2·29	2·24	*	1·0	0·89	0·62	0·62	0·29	0·29
18	1·99	1·51	2·76	3·11	0·56	0·81	1·0	0·88	0·36	0·47	0·81	0·68
19	1·41	2·76	2·52	3·02	1·29	2·24	1·0	0·88	0·54	0·88	0·87	0·70
20	1·02	2·76	2·10	2·12	1·77	2·24	1·0	0·88	0·63	0·85	0·69	0·56
21	2·76	1·76	2·13	3·45	2·24	2·48	1·0	0·85	0·32	0·95	0·87	0·76
22	2·13	1·76	1·61	2·76	1·33	2·48	1·0	0·81	0·54	0·86	0·78	0·70
23	2·13	1·58	1·82	2·50	1·33	1·59	1·0	0·78	0·55	0·76	0·76	0·68
24	1·47	1·76	1·89	2·05	*	2·48	1·0	0·74	0·67	0·77	0·66	0·61
25	1·90	0·01	1·77	2·60	0·22	2·52	−1·0	0·28	0·31	0·31	0·40	0·40
26	1·41	1·76	1·92	3·10	1·29	2·48	1·0	0·72	0·52	0·77	0·69	0·61
27	1·18	1·76	1·80	1·84	1·09	2·48	1·0	0·71	0·63	0·73	0·58	0·55
28	1·16	1·76	1·80	1·87	0·99	2·48	1·0	0·71	0·63	0·72	0·58	0·55
29	1·00	1·76	1·80	2·24	*	2·48	1·0	0·70	0·64	0·71	0·55	0·53
30	0·56	1·76	1·68	3·02	*	2·48	1·0	0·66	0·60	0·64	0·45	0·45

$E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{h}+\mathbf{k}+2\mathbf{l}}$ is positive. Using the Gram–Charlier expansion of the characteristic function we obtain

$$P_+ \simeq 0{\cdot}5 + 0{\cdot}5 \tanh\left(\frac{R_1R_2R_3}{N\sqrt{N}}\frac{A_1 + A_2 + A_3}{1 + B_1 + B_2}\right), \qquad (10)$$

where

$$\begin{aligned}
A_1 &= \varepsilon_4\varepsilon_7\varepsilon_8 + \varepsilon_5\varepsilon_6\varepsilon_9 + \varepsilon_5\varepsilon_7\varepsilon_{13} + \varepsilon_4\varepsilon_6\varepsilon_{11} + \varepsilon_4\varepsilon_5\varepsilon_{10} \\
&\quad + \varepsilon_6\varepsilon_7\varepsilon_{12} + \varepsilon_4\varepsilon_5\varepsilon_6 + \varepsilon_4\varepsilon_5\varepsilon_7 + \varepsilon_4\varepsilon_6\varepsilon_7 + \varepsilon_5\varepsilon_6\varepsilon_7 \\
&\quad + \tfrac{1}{2}[\varepsilon_4\varepsilon_{14}(\varepsilon_8 + \varepsilon_{10} + \varepsilon_{11}) + \varepsilon_5\varepsilon_{15}(\varepsilon_9 + \varepsilon_{10} + \varepsilon_{13}) \\
&\quad + \varepsilon_6\varepsilon_{16}(\varepsilon_9 + \varepsilon_{11} + \varepsilon_{12}) + \varepsilon_7\varepsilon_{17}(\varepsilon_8 + \varepsilon_{12} + \varepsilon_{13})], \\
A_2 &= \varepsilon_4\varepsilon_5 + \varepsilon_6\varepsilon_7 + \varepsilon_4\varepsilon_6 + \varepsilon_5\varepsilon_7 + \varepsilon_4\varepsilon_7 + \varepsilon_5\varepsilon_6 \\
&\quad + \tfrac{1}{2}[\varepsilon_4(\varepsilon_8 + \varepsilon_{10} + \varepsilon_{11} + \varepsilon_{14}) + \varepsilon_5(\varepsilon_9 + \varepsilon_{10} + \varepsilon_{13} \\
&\quad + \varepsilon_{15}) + \varepsilon_6(\varepsilon_9 + \varepsilon_{11} + \varepsilon_{12} + \varepsilon_{16}) \\
&\quad + \varepsilon_7(\varepsilon_8 + \varepsilon_{12} + \varepsilon_{13} + \varepsilon_{17})], \\
A_3 &= \tfrac{1}{2}(\varepsilon_4 + \varepsilon_5 + \varepsilon_6 + \varepsilon_7), \\
B_1 &= (\varepsilon_1\varepsilon_2\varepsilon_8 + \varepsilon_1\varepsilon_2\varepsilon_9 + \varepsilon_1\varepsilon_3\varepsilon_{13} + \varepsilon_1\varepsilon_3\varepsilon_{11} + \varepsilon_1\varepsilon_4\varepsilon_5 \\
&\quad + \varepsilon_1\varepsilon_6\varepsilon_7 + \varepsilon_1\varepsilon_{10}\varepsilon_{15} + \varepsilon_1\varepsilon_{10}\varepsilon_{14} + \varepsilon_1\varepsilon_{12}\varepsilon_{17} \\
&\quad + \varepsilon_1\varepsilon_{12}\varepsilon_{16} + \varepsilon_2\varepsilon_3\varepsilon_{10} + \varepsilon_2\varepsilon_3\varepsilon_{12} + \varepsilon_2\varepsilon_4\varepsilon_6 \\
&\quad + \varepsilon_2\varepsilon_5\varepsilon_7 + \varepsilon_2\varepsilon_{11}\varepsilon_{16} + \varepsilon_2\varepsilon_{11}\varepsilon_{14} + \varepsilon_2\varepsilon_{13}\varepsilon_{17})], \\
&\quad + \varepsilon_2\varepsilon_{13}\varepsilon_{15} + \varepsilon_3\varepsilon_4\varepsilon_7 + \varepsilon_3\varepsilon_5\varepsilon_6 + \varepsilon_3\varepsilon_8\varepsilon_{14} \\
&\quad + \varepsilon_3\varepsilon_8\varepsilon_{17} + \varepsilon_3\varepsilon_9\varepsilon_{15} + \varepsilon_3\varepsilon_9\varepsilon_{16} + \varepsilon_4\varepsilon_5\varepsilon_{10} \\
&\quad + \varepsilon_4\varepsilon_6\varepsilon_{11} + \varepsilon_4\varepsilon_7\varepsilon_8 + \varepsilon_5\varepsilon_6\varepsilon_9 + \varepsilon_5\varepsilon_7\varepsilon_{13} \\
&\quad + \varepsilon_6\varepsilon_7\varepsilon_{12} + \varepsilon_8\varepsilon_{10}\varepsilon_{13} + \varepsilon_8\varepsilon_{11}\varepsilon_{12} + \varepsilon_9\varepsilon_{10}\varepsilon_{11} \\
&\quad + \varepsilon_9\varepsilon_{12}\varepsilon_{13})/2N, \\
B_2 &= \{-\sum_{i=1}^{17} H_4(R_i) + H_4(R_4)\varepsilon_{14} + H_4(R_5)\varepsilon_{15} \\
&\quad + H_4(R_6)\varepsilon_{16} + H_4(R_7)\varepsilon_{17}\}/8N, \\
\varepsilon_i &= (E_i^2 - 1).
\end{aligned}$$

The number of the three-phase seminvariants for which all the seventeen reflexions are in the measurements may be a small percentage of the observable three-phase seminvariants. In these cases the probability values can be easily derived from (3) by making equal to unity the terms ε_i corresponding to the magnitudes R_i which are not in the measurements and by making equal to zero the respective $H_4(R_i)$'s. The practical applications of (10) are satisfactory and are described by Burla, Polidori, Nunzi & Giacovazzo (1977).

5. Conclusions

The conditional joint probability distributions of the two and three-phases structure seminvariants in $P\bar{1}$, given the magnitudes belonging to their first phasing shells, have been found. As anticipated in the earlier work, the concept of representation of a structure seminvariant plays an essential role. We have shown here that the application of the theory of representations enables us to generalize the coincidence method of Grant, Howells & Rogers (1957). The extension of this theory to all the space groups is the object of a subsequent paper.

The author wishes to thank Mr G. Cascarano who performed the calculations shown in Table 1. This research was supported by the Consiglio Nazionale delle Ricerche, grant No. 75.1066.05.115.4593.

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