$$\prod_{\lambda=1}^{N/2} g_\lambda = \exp\left\{-\tfrac{1}{2}(\sigma_1^2+\sigma_2^2+\sigma_3^2+\sigma_4^2+\sigma_{12}^2+\sigma_{23}^2+\sigma_{31}^2)\right.$$
$$-\frac{i}{N^{1/2}}(\sigma_1\sigma_4\sigma_{23}+\sigma_1\sigma_3\sigma_{31}+\sigma_1\sigma_2\sigma_{12}+\sigma_2\sigma_3\sigma_{23}$$
$$+\sigma_2\sigma_4\sigma_{31}+\sigma_3\sigma_4\sigma_{12})$$
$$+\frac{1}{N}(\sigma_1\sigma_2\sigma_3\sigma_4+\sigma_2\sigma_3\sigma_{31}\sigma_{12}+\sigma_2\sigma_4\sigma_{12}\sigma_{23}+\sigma_3\sigma_4\sigma_{23}\sigma_{31}$$
$$\left.+\sigma_1\sigma_4\sigma_{31}\sigma_{12}+\sigma_1\sigma_3\sigma_{12}\sigma_{23}+\sigma_1\sigma_2\sigma_{23}\sigma_{31})\right\}$$
$$\times\left\{1+O\left(\frac{1}{N}\right)\right\} \qquad (II.1)$$

where $O(1/N)$ represents the terms of order $1/N$ or higher in which the terms of order $1/N$ contain only even powers of the σ's.

APPENDIX III

Evaluating the sevenfold integral (2.3)

III. 1. *The σ_1 integration*

Substitute for $\prod_{\lambda=1}^{N/2} g_\lambda$ from (II.I) into (2.3), combine the terms in the exponent involving σ_1, complete the square, and perform the σ_1 integration.

III. 2. *The remaining integrations*

One continues in this way, carrying out the successive integrations with respect to $\sigma_2, \sigma_3, \ldots$, until finally (2.5) is obtained.

It is instructive to compare these integrations with those of the earlier paper (Appendix IV).

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Conditional Probability Distributions of the Four-Phase Structure Invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in $P\bar{1}$*

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A crystal structure in $P\bar{1}$ is assumed to be fixed and the seven non-negative numbers R_1, R_2, R_3, R_4, R_{12}, R_{23}, R_{31} are also given. It is assumed that **h**,**k**,**l**,**m** are random variables uniformly and independently distributed over the subsets of reciprocal space defined by

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4, \qquad (1)$$

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12},\ |E_{\mathbf{k}+\mathbf{l}}|=R_{23},\ |E_{\mathbf{l}+\mathbf{h}}|=R_{31}, \qquad (2)$$

and

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,. \qquad (3)$$

Then the structure invariant

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \qquad (4)$$

is a function of the primitive random variables **h**,**k**,**l**,**m**. The conditional probability distribution of φ, given (1) and (2), is obtained and compared with the conditional probability distribution of φ when only (1) is given. Some calculations are presented which show the usefulness of the distribution, given (1) and (2), in estimating the value of φ.

1. Introduction

The methods introduced in two previous papers (Hauptman 1975*a*, *b*) for $P1$ are applied here to the space group $P\bar{1}$. Again, as in the earlier work, the joint probability distribution of seven structure factors [Green & Hauptman, 1976, equation (2.5)] leads directly to the conditional probability distribution of the four-phase structure invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, given the seven magnitudes $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{h}+\mathbf{k}}|$, $|E_{\mathbf{k}+\mathbf{l}}|$, $|E_{\mathbf{l}+\mathbf{h}}|$. However, in contrast to the earlier distri-

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bution which is continuous, the distribution to be derived here is discrete because the structure invariant has only the two possible values, 0 or π.

2. The joint conditional probability distribution of the four phases $\varphi_{\mathbf{h}}, \varphi_{\mathbf{k}}, \varphi_{\mathbf{l}}, \varphi_{\mathbf{m}}$, given the seven magnitudes, $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{h+k}}|, |E_{\mathbf{k+l}}|, |E_{\mathbf{l+h}}|$

Suppose that a crystal structure consisting of N identical atoms per unit cell in the space group $P\bar{1}$ is specified and that the seven non-negative numbers $R_1, R_2, R_3, R_4, R_{12}, R_{23}, R_{31}$ are also fixed. Denote by $\varphi_{\mathbf{h}}$ the phase of the normalized structure factor $E_{\mathbf{h}}$. Define the fourfold Cartesian product $W\times W\times W\times W$ of reciprocal space W with itself to consist of the collection of all ordered quadruples $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$ of reciprocal vectors $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$. Suppose finally that the ordered quadruple $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$ of reciprocal vectors is a random variable which is uniformly distributed over the subset of the Cartesian product $W\times W\times W\times W$ for which

$$|E_{\mathbf{h}}|=R_1,\ |E_{\mathbf{k}}|=R_2,\ |E_{\mathbf{l}}|=R_3,\ |E_{\mathbf{m}}|=R_4, \tag{2.1}$$

$$|E_{\mathbf{h+k}}|=R_{12},\ |E_{\mathbf{k+l}}|=R_{23},\ |E_{\mathbf{l+h}}|=R_{31}, \tag{2.2}$$

and

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0\,. \tag{2.3}$$

[Strictly speaking, in order to insure that the range of the primitive random variable $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$ be non-vacuous, it is necessary, for example, to replace the equality $|E_{\mathbf{h}}|=R_1$ of (2.1) by the inequalities $R_1\le|E_{\mathbf{h}}|\le R_1+\mathrm{d}R_1$, where $\mathrm{d}R_1$ is a 'small' positive number, *etc.*]. In view of (2.1)–(2.3), the random variables $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$, the components of the ordered quadruple $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$, are not independently distributed in reciprocal space. Then $\varphi_{\mathbf{h}},\varphi_{\mathbf{k}},\varphi_{\mathbf{l}},\varphi_{\mathbf{m}}$, the phases of the normalized structure factors $E_{\mathbf{h}},E_{\mathbf{k}},E_{\mathbf{l}},E_{\mathbf{m}}$, as functions of the primitive random variables $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$, are themselves random variables. Denote by $P(\Phi_1, \Phi_2, \Phi_3, \Phi_4\,|\,R_1, R_2, R_3, R_4, R_{12}, R_{23}, R_{31})$ the joint conditional probability distribution of the four phases $\varphi_{\mathbf{h}},\varphi_{\mathbf{k}},\varphi_{\mathbf{l}},\varphi_{\mathbf{m}}$, given (2.1), (2.2) and (2.3). Then $P(\Phi_1,\Phi_2,\Phi_3,\Phi_4\,|\,R_1,R_2,R_3,R_4,R_{12},R_{23},R_{31})$ is found from (2.5) of the previous paper (Green & Hauptman, 1976) by fixing the magnitudes of $S_1, S_2, S_3, S_4, S_{12}, S_{23}, S_{31}$ in accordance with the scheme

$$|S_1|=R_1,\ |S_2|=R_2,\ |S_3|=R_3,\ |S_4|=R_4, \tag{2.4}$$

$$|S_{12}|=R_{12},\ |S_{23}|=R_{23},\ |S_{31}|=R_{31}, \tag{2.5}$$

i.e.

$$S_1=R_1\cos\Phi_1,\ S_2=R_2\cos\Phi_2,\ S_3=R_3\cos\Phi_3,\ S_4=R_4\cos\Phi_4, \tag{2.6}$$

$$S_{12}=R_{12}\cos\Phi_{12},\ S_{23}=R_{23}\cos\Phi_{23},\ S_{31}=R_{31}\cos\Phi_{31}, \tag{2.7}$$

where Φ_{12} is the variable associated with the phase $\varphi_{\mathbf{h+k}}$, *etc.*, summing with respect to S_{12}, S_{23}, S_{31} over their two possible signs (+ and −) or, equivalently, summing with respect to $\Phi_{12},\Phi_{23},\Phi_{31}$ over their two possible values (0 and π), and multiplying the result by a suitable normalizing factor. Carrying out these summations one finally obtains, correct up to and including terms of order $1/N$ [since $O(1/N)$ of the previous paper consists of all terms of order $1/N$ or higher in which the terms of order $1/N$ contain only even powers of the S's],

$$P(\Phi_1,\Phi_2,\Phi_3,\Phi_4\,|\,R_1,R_2,R_3,R_4,R_{12},R_{23},R_{31}) \simeq \frac{1}{K}\exp\{-B\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4)\} \times\cosh\frac{R_{12}Y_{12}}{N^{1/2}}\cosh\frac{R_{23}Y_{23}}{N^{1/2}}\cosh\frac{R_{31}Y_{31}}{N^{1/2}} \tag{2.8}$$

where

$$B=\frac{2}{N}R_1R_2R_3R_4, \tag{2.9}$$

$$Y_{12}=[R_1^2R_2^2+R_3^2R_4^2+2R_1R_2R_3R_4\times\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4)]^{1/2}, \tag{2.10}$$

$$Y_{23}=[R_2^2R_3^2+R_1^2R_4^2+2R_1R_2R_3R_4\times\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4)]^{1/2}, \tag{2.11}$$

$$Y_{31}=[R_3^2R_1^2+R_2^2R_4^2+2R_1R_2R_3R_4\times\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4)]^{1/2}, \tag{2.12}$$

and K is a suitable normalizing constant, independent of $\Phi_1,\Phi_2,\Phi_3,\Phi_4$. Although K is readily found by summing (2.8) over the 16 sets of values of $\Phi_1,\Phi_2,\Phi_3,\Phi_4$ and setting the result equal to unity, the value of this normalizing factor is not needed for the present purpose and is therefore not derived explicitly. Equations (2.8)–(2.12) should be compared with equations (2.5)–(2.9) of the earlier work in $P1$ (Hauptman, 1975*b*), but it should be emphasized again that the present distribution (2.8) is discrete since each of $\Phi_1, \Phi_2, \Phi_3, \Phi_4$ takes on only the two values $0,\pi$.

It is clear from (2.8)–(2.12) that the distribution (2.8) is a function of the sum $\Phi=\Phi_1+\Phi_2+\Phi_3+\Phi_4$. Hence (2.8) leads directly to the conditional distribution, given (2.1) and (2.2), of the sum $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, as is shown next.

3. The conditional probability distribution of the structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, given the seven magnitudes $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{h+k}}|, |E_{\mathbf{k+l}}|, |E_{\mathbf{l+h}}|$

Using the same hypotheses as in §2, the structure invariant

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}} \tag{3.1}$$

is a random variable whose conditional probability distribution, given (2.1) and (2.2), $P(\Phi\,|\,R_1, R_2, R_3, R_4, R_{12}, R_{23}, R_{31})$, is readily found from (2.8)–(2.12). Thus, correct up to and including terms of order $1/N$, the major result of this paper is given by

$$P(\Phi|R_1,R_2,R_3,R_4,R_{12},R_{23},R_{31}) \simeq \frac{1}{L}\exp(-B\cos\Phi) \times \cosh\frac{R_{12}Z_{12}}{N^{1/2}}\cosh\frac{R_{23}Z_{23}}{N^{1/2}}\cosh\frac{R_{31}Z_{31}}{N^{1/2}} \quad (3.2)$$

where B is defined by (2.9),

$$Z_{12}=[R_1^2R_2^2+R_3^2R_4^2+2R_1R_2R_3R_4\cos\Phi]^{1/2}, \quad (3.3)$$

$$Z_{23}=[R_2^2R_3^2+R_1^2R_4^2+2R_1R_2R_3R_4\cos\Phi]^{1/2}, \quad (3.4)$$

$$Z_{31}=[R_3^2R_1^2+R_2^2R_4^2+2R_1R_2R_3R_4\cos\Phi]^{1/2}, \quad (3.5)$$

and the normalizing constant L is readily found to be

$$L=\exp(-B)\cosh\frac{R_{12}Z_{12}^{+}}{N^{1/2}}\cosh\frac{R_{23}Z_{23}^{+}}{N^{1/2}}\cosh\frac{R_{31}Z_{31}^{+}}{N^{1/2}} +\exp(B)\cosh\frac{R_{12}Z_{12}^{-}}{N^{1/2}}\cosh\frac{R_{23}Z_{23}^{-}}{N^{1/2}}\cosh\frac{R_{31}Z_{31}^{-}}{N^{1/2}}, \quad (3.6)$$

where

$$Z_{12}^{\pm}=R_1R_2\pm R_3R_4, \quad (3.7)$$

$$Z_{23}^{\pm}=R_2R_3\pm R_1R_4, \quad (3.8)$$

$$Z_{31}^{\pm}=R_3R_1\pm R_2R_4, \quad (3.9)$$

and the upper (lower) signs go together.

If one denotes by $P_+(P_-)$ the conditional probability, given (2.1) and (2.2), that

$$\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}=0\ (\pi), \quad (3.10)$$

or that

$$\cos\varphi=+1\ (-1), \quad (3.11)$$

or that

$$E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{l}}E_{\mathbf{m}} \text{ be positive (negative)}, \quad (3.12)$$

then (3.2) is replaced by the more suggestive

$$P_{\pm}\simeq\frac{1}{L}\exp(\mp B)\cosh\frac{R_{12}Z_{12}^{\pm}}{N^{1/2}} \times\cosh\frac{R_{23}Z_{23}^{\pm}}{N^{1/2}}\cosh\frac{R_{31}Z_{31}^{\pm}}{N^{1/2}}, \quad (3.13)$$

where the upper (lower) signs go together and $L, Z_{12}^{\pm}, Z_{23}^{\pm}, Z_{31}^{\pm}$ are given by (3.6)–(3.9).

The similarity between (3.2) and (3.13) with the major result of the earlier work in $P1$ [equation (3.2), Hauptman, 1975*b*] is noteworthy. However, it must be stressed again that the present distributions are discrete, *i.e.* Φ must be 0 or π, while the earlier distribution is continuous.

It should be observed finally that P_+ may lie anywhere between 0 and 1; P_+ is close to 0 or close to 1 according as R_{12}, R_{23}, R_{31} are all relatively small or all relatively large respectively.

3.1. *The conditional expected value and conditional variance of* $\cos\varphi$

It is clear from (3.13) that the conditional expected value of $\cos\varphi$, given (2.1) and (2.2), is simply

$$\epsilon=\epsilon(\cos\varphi)=\epsilon(\cos\varphi|R_1,R_2,R_3,R_4,R_{12},R_{23},R_{31}) \simeq P_+-P_-. \quad (3.14)$$

Likewise the conditional variance of $\cos\varphi$, given (2.1) and (2.2), is found from (3.14) to be

$$\sigma^2=\sigma^2(\cos\varphi|R_1,R_2,R_3,R_4,R_{12},R_{23},R_{31}) \simeq\epsilon(\cos^2\varphi)-[\epsilon(\cos\varphi)]^2=4P_+P_-. \quad (3.15)$$

It follows from (3.15) that the conditional standard deviation is given by

$$\sigma=2\sqrt{P_+P_-}. \quad (3.16)$$

3.2. *The special case* $|E_{\mathbf{h}+\mathbf{k}}|\simeq|E_{\mathbf{k}+\mathbf{l}}|\simeq|E_{\mathbf{l}+\mathbf{h}}|\simeq 0$

In the case that

$$|E_{\mathbf{h}+\mathbf{k}}|=R_{12}\simeq 0, \quad (3.17)$$

$$|E_{\mathbf{k}+\mathbf{l}}|=R_{23}\simeq 0, \quad (3.18)$$

$$|E_{\mathbf{l}+\mathbf{h}}|=R_{31}\simeq 0, \quad (3.19)$$

(3.13) is replaced by

$$P_{\pm}(|R_{12}\simeq R_{23}\simeq R_{31}\simeq 0)\simeq\frac{1}{L}\exp(\mp B) \quad (3.20)$$

where

$$L=2\cosh B \quad (3.21)$$

so that, in this special case, $P_+<\frac{1}{2}$, φ is probably equal to π, and the larger the value of B the more likely it is that $\varphi=\pi$.

4. The conditional probability distribution of the structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$, given the four magnitudes $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$

If, instead of being given the seven magnitudes (2.1) and (2.2), one is given only the four magnitudes (2.1), then the conditional probability distribution of φ, given (2.1), is found from (3.1) of the previous paper (Green & Hauptman, 1976) to be, correct up to and including terms of order $1/N$,

$$P_{\pm}(4)\simeq\frac{1}{M}\exp\left(\pm\frac{B}{2}\right), \quad (4.1)$$

where

$$M=2\cosh\frac{B}{2}, \quad (4.2)$$

and $P_+(4)[P_-(4)]$ is the conditional probability, given (2.1), that

$$\varphi=0\ (\pi) \quad (4.3)$$

or that

$$\cos\varphi=+1\ (-1). \quad (4.4)$$

Equation (4.1) should be compared with equation (4.1) of the earlier work in $P1$ (Hauptman, 1975*b*). Particularly noteworthy is the comparison of (4.1) with (3.20) which illustrates with particular force the dramatic change which may take place when all seven magnitudes (2.2) and (2.1) are assumed to be given instead of merely the four magnitudes (2.1). In sharp contrast to (3.20), $P_+(4)>\frac{1}{2}$, φ now is probably equal to 0, and the larger the value of B the more likely it is that $\varphi=0$.

5. The applications

A crystal structure in $P\bar{1}$ consisting of $N=90$ identical atoms in the unit cell was constructed and 6701 normalized structure factors $E_{\mathbf{h}}$ calculated. Using the $299|E|$'s >2 (*i.e.* $|E_{\mathbf{h}}|>2$, $|E_{\mathbf{k}}|>2$, $|E_{\mathbf{l}}|>2$, $|E_{\mathbf{m}}|>2$) the 1000 quartets

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0 \qquad (5.1)$$

were constructed having the largest values of B. The 1000 values of P_+, equation (3.13), and of the standard deviation σ, equation (3.16), were calculated and these are shown in Table 1* arranged in increasing order of the standard deviation (SIG). The column headed cos (T) lists the true values of cos φ. The three special invariants with serial numbers 522, 634, 698 do not obey the distribution law (3.13), since $\mathbf{h}=\mathbf{k}$, and these are therefore not considered further. It is noteworthy that the first discrepancy in the table occurs at invariant 786. Thus the first 782 invariants are calculated with perfect accuracy and, of these, 745 are equal to 0 and 37 equal to π. The preponderance of 0 values is a consequence of equation (4.1) since small values of σ are correlated with large values of B which, in view of (4.1), implies that φ is probably equal to 0. Toward the end of Table 1, as P_+ values tend toward $\frac{1}{2}$, one observes increasing numbers of incorrect indications. Naturally, in the applications, one would not use the latter invariants since, in view of the large standard deviations, they are known not to be reliably determined. It is noteworthy that the estimates are somewhat more reliable than the values of P_+ appear to indicate, at least for the smaller values of σ. This is probably due to the fact that (3.13) is correct to terms of order $1/N$ only, and the ability to take into account terms of order higher than $1/N$ would probably lead to a more accurate formula for P_+, at least for the larger values of B. Toward the end of Table 1, where σ values are large and B values tend to be small, (3.13) appears to yield more accurate values of P_+ since here one observes the expected fraction of correct estimates as indicated by the value of P_+.

* Only 50 entries are shown here. The full table has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31305 (20 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *1000 values of* P_+, *equation* (3.13), *and* σ, *equation* (3.16), *for a structure in* $P\bar{1}$ *consisting of* $N=90$ *identical atoms in the unit cell*

					Observed Magnitudes, |E|										
No.	$\vec{h}$	$\vec{k}$	$\vec{l}$	$\vec{m}$	$\vec{h}$	$\vec{k}$	$\vec{l}$	$\vec{m}$	$\vec{h}+\vec{k}$	$\vec{k}+\vec{l}$	$\vec{l}+\vec{h}$	P	COS(T)	P(+)	SIG
6	8 $\bar{10}$ 0	$\bar{3}$ $\bar{6}$ 3	$\bar{4}$ 6 $\bar{8}$	$\bar{1}$ 10 5	3.68	2.95	2.81	2.39	3.00	4.25	3.56	1.62	0.999	0.999	0.002
7	4 $\bar{4}$ $\bar{8}$	$\bar{2}$ 11 0	1 $\bar{1}$ 5	$\bar{3}$ $\bar{6}$ 3	3.56	3.46	3.39	2.95	4.17	2.39	2.41	2.74	0.999	0.999	0.003
8	2 $\bar{11}$ 0	6 1 0	1 $\bar{1}$ 5	$\bar{9}$ 11 $\bar{5}$	3.46	3.44	3.39	2.64	3.68	4.25	1.56	2.36	0.999	0.999	0.003
9	1 12 0	$\bar{6}$ $\bar{1}$ 0	$\bar{3}$ 0 1	8 $\bar{11}$ $\bar{1}$	3.66	3.44	2.99	2.35	2.77	3.72	3.70	1.96	0.999	0.999	0.003
10	2 7 $\bar{8}$	2 $\bar{11}$ 0	2 6 7	$\bar{6}$ $\bar{2}$ 1	4.17	3.46	3.33	2.23	3.56	4.18	1.50	2.38	0.999	0.999	0.007
186	2 7 $\bar{8}$	7 $\bar{6}$ 7	$\bar{6}$ 2 3	$\bar{3}$ $\bar{3}$ $\bar{2}$	4.17	3.36	3.00	2.44	3.72	1.19	2.14	2.27	0.999	0.998	0.074
187	2 7 $\bar{8}$	$\bar{9}$ $\bar{1}$ 1	8 $\bar{11}$ $\bar{1}$	$\bar{1}$ 5 8	4.17	3.72	2.35	2.34	3.36	3.66	0.26	1.89	0.999	0.998	0.074
188	4 $\bar{5}$ 7	$\bar{6}$ 2 3	7 $\bar{7}$ $\bar{10}$	$\bar{5}$ 10 0	4.18	3.00	2.68	2.28	1.49	3.96	1.35	1.71	0.999	0.998	0.074
189	1 12 0	6 $\bar{2}$ $\bar{3}$	$\bar{3}$ 0 1	$\bar{4}$ $\bar{10}$ 2	3.66	3.00	2.99	2.22	2.19	1.33	3.70	1.63	0.999	0.998	0.074
190	4 $\bar{5}$ 7	3 0 $\bar{1}$	1 11 0	$\bar{8}$ $\bar{6}$ $\bar{6}$	4.18	2.99	2.76	2.03	1.89	3.02	2.30	1.55	0.999	0.998	0.075
401	1 $\bar{5}$ $\bar{7}$	7 1 4	2 1 0	$\bar{10}$ 3 3	3.96	3.12	2.58	2.38	1.96	1.32	2.67	1.69	1.000	0.991	0.179
402	4 $\bar{5}$ 7	$\bar{7}$ 9 0	$\bar{3}$ $\bar{1}$ 0	6 $\bar{3}$ $\bar{7}$	4.18	2.63	2.61	2.57	2.67	1.33	2.03	1.63	0.999	0.991	0.181
403	8 $\bar{10}$ 0	1 $\bar{1}$ 5	$\bar{5}$ 11 0	$\bar{4}$ 0 $\bar{5}$	3.68	3.39	2.77	2.09	2.64	0.97	2.61	1.60	0.999	0.991	0.181
404	1 $\bar{1}$ 5	1 $\bar{7}$ 7	6 $\bar{3}$ $\bar{9}$	$\bar{8}$ 11 $\bar{3}$	3.39	3.04	2.77	2.46	1.97	1.50	2.31	1.56	0.999	0.991	0.182
405	7 0 5	$\bar{1}$ $\bar{11}$ 0	2 0 $\bar{2}$	$\bar{8}$ 11 $\bar{3}$	4.25	2.76	2.55	2.46	3.32	0.68	2.23	1.63	0.999	0.991	0.183
566	4 $\bar{5}$ 7	$\bar{5}$ 6 $\bar{7}$	3 9 $\bar{1}$	$\bar{2}$ $\bar{10}$ 1	4.18	3.02	2.56	2.51	0.24	0.10	0.06	1.81	-1.000	0.029	0.339
567	7 0 5	$\bar{8}$ 10 0	3 0 $\bar{10}$	$\bar{2}$ $\bar{10}$ 5	4.25	3.68	2.37	2.21	2.39	1.38	1.72	1.82	0.999	0.970	0.340
568	4 $\bar{5}$ 7	$\bar{8}$ 9 1	3 1 0	1 $\bar{5}$ $\bar{8}$	4.18	2.84	2.61	2.34	3.56	1.59	0.09	1.61	0.999	0.970	0.340
569	1 $\bar{1}$ 5	3 10 $\bar{6}$	7 $\bar{9}$ 0	$\bar{11}$ 0 1	3.39	3.16	2.63	2.51	1.35	1.53	2.09	1.56	0.999	0.970	0.340
570	4 $\bar{4}$ $\bar{8}$	$\bar{6}$ $\bar{1}$ 0	$\bar{5}$ 2 8	7 3 0	3.56	3.44	3.17	2.31	0.04	0.49	0.21	1.99	-0.999	0.030	0.342
636	1 $\bar{5}$ $\bar{7}$	$\bar{6}$ $\bar{1}$ 0	1 $\bar{7}$ 7	4 13 0	3.96	3.44	3.04	2.40	2.30	0.07	2.33	2.21	0.999	0.952	0.423
637	7 0 5	$\bar{3}$ $\bar{4}$ $\bar{7}$	3 6 $\bar{3}$	$\bar{7}$ $\bar{2}$ 5	4.25	3.00	2.95	2.26	0.01	0.38	0.58	1.89	-1.000	0.047	0.423
638	9 1 $\bar{1}$	3 0 $\bar{1}$	$\bar{4}$ $\bar{8}$ 8	$\bar{8}$ 7 $\bar{6}$	3.72	2.99	2.80	2.36	1.25	1.04	2.51	1.63	0.999	0.952	0.423
639	10 $\bar{5}$ $\bar{1}$	3 0 $\bar{1}$	$\bar{10}$ 11 $\bar{2}$	$\bar{3}$ $\bar{6}$ 4	3.26	2.99	2.77	2.64	2.68	1.34	0.66	1.59	0.999	0.953	0.423
640	4 $\bar{5}$ 7	$\bar{7}$ 6 $\bar{7}$	$\bar{2}$ $\bar{10}$ 1	5 9 $\bar{1}$	4.18	3.36	2.51	2.05	0.29	0.19	0.10	1.60	-0.999	0.047	0.424
641	8 $\bar{10}$ 0	1 $\bar{1}$ 5	$\bar{9}$ $\bar{2}$ 1	0 13 $\bar{6}$	3.68	3.39	2.77	2.15	2.64	0.49	1.90	1.65	0.999	0.951	0.427
642	9 1 $\bar{1}$	$\bar{2}$ 11 0	$\bar{4}$ $\bar{11}$ 1	$\bar{3}$ $\bar{1}$ 0	3.72	3.46	3.02	2.61	1.14	1.17	2.28	2.25	0.999	0.951	0.430
643	2 $\bar{12}$ $\bar{1}$	$\bar{8}$ 10 0	3 $\bar{1}$ $\bar{1}$	3 3 2	3.70	3.68	2.67	2.44	0.14	0.62	0.43	1.96	-0.999	0.049	0.434
644	9 1 $\bar{1}$	$\bar{1}$ $\bar{12}$ 0	0 4 7	$\bar{8}$ 7 $\bar{6}$	3.72	3.66	2.45	2.36	2.35	1.04	1.61	1.75	0.999	0.950	0.435
645	1 9 $\bar{7}$	2 $\bar{11}$ 0	$\bar{6}$ $\bar{1}$ 0	3 3 7	3.54	3.46	3.44	2.26	0.28	0.47	0.68	2.12	-0.999	0.050	0.439
781	2 7 $\bar{8}$	3 0 $\bar{1}$	2 1 0	$\bar{7}$ $\bar{8}$ 9	4.17	2.99	2.58	2.22	0.74	0.68	2.80	1.59	1.000	0.871	0.670
782	7 0 5	$\bar{9}$ $\bar{1}$ 1	2 $\bar{12}$ $\bar{1}$	0 13 $\bar{5}$	4.25	3.72	3.70	2.05	1.49	1.54	1.46	2.66	0.999	0.869	0.673
783	6 $\bar{6}$ 7	$\bar{6}$ $\bar{1}$ 0	3 0 $\bar{1}$	$\bar{3}$ 7 $\bar{6}$	3.57	3.44	2.99	2.08	1.42	1.25	1.51	1.69	0.999	0.867	0.677
784	9 1 $\bar{1}$	1 $\bar{7}$ 7	$\bar{5}$ 3 $\bar{8}$	$\bar{5}$ 3 2	3.72	3.04	2.99	2.07	2.08	0.83	1.35	1.55	0.999	0.867	0.678
785	2 7 $\bar{8}$	7 1 4	$\bar{3}$ $\bar{6}$ 4	$\bar{6}$ $\bar{2}$ 0	4.17	3.12	2.64	2.06	0.86	0.58	0.14	1.57	-1.000	0.133	0.680
786	7 0 5	$\bar{3}$ $\bar{10}$ 6	$\bar{7}$ 9 0	3 1 $\bar{11}$	4.25	3.16	2.63	2.18	1.18	1.53	1.45	1.71	-1.000	0.865	0.681
787	2 7 $\bar{8}$	6 1 0	$\bar{9}$ $\bar{2}$ 1	1 $\bar{6}$ 7	4.17	3.44	2.77	2.03	0.20	1.79	1.93	1.79	0.999	0.865	0.683
788	2 $\bar{11}$ 0	1 $\bar{1}$ 5	$\bar{6}$ 2 3	3 10 $\bar{8}$	3.46	3.39	3.00	2.43	1.56	1.23	1.28	1.90	0.999	0.863	0.686
789	6 1 0	0 9 $\bar{8}$	$\bar{8}$ $\bar{9}$ 8	2 $\bar{1}$ 0	3.44	3.05	2.70	2.55	0.81	0.76	2.38	1.60	0.999	0.860	0.693
790	4 $\bar{5}$ 7	$\bar{6}$ $\bar{1}$ 0	8 5 $\bar{10}$	$\bar{6}$ 1 3	4.18	3.44	2.54	2.24	1.39	1.26	1.52	1.81	0.999	0.859	0.694
881	2 7 $\bar{8}$	$\bar{4}$ 4 8	3 3 2	$\bar{1}$ $\bar{14}$ $\bar{2}$	4.17	3.56	2.44	2.12	3.46	0.54	0.50	1.70	0.999	0.763	0.860
882	4 $\bar{5}$ 7	6 $\bar{3}$ $\bar{9}$	$\bar{8}$ 7 2	$\bar{2}$ 1 0	4.18	2.77	2.59	2.55	1.52	0.25	0.36	1.70	-0.999	0.238	0.852
883	1 $\bar{5}$ $\bar{7}$	$\bar{3}$ 0 1	0 11 $\bar{2}$	2 $\bar{6}$ 8	3.96	2.99	2.65	2.30	0.97	0.50	2.18	1.60	1.000	0.760	0.853
884	1 $\bar{8}$ 7	5 $\bar{2}$ $\bar{8}$	$\bar{8}$ 9 1	2 1 0	3.29	3.17	2.84	2.58	0.94	0.75	0.56	1.70	-1.000	0.243	0.858
885	8 $\bar{10}$ 0	$\bar{1}$ 1 $\bar{5}$	$\bar{6}$ $\bar{5}$ 6	$\bar{1}$ 14 $\bar{1}$	3.68	3.39	2.50	2.28	0.69	1.00	0.50	1.58	-1.000	0.246	0.861
886	7 0 5	$\bar{8}$ $\bar{9}$ 4	3 1 0	$\bar{2}$ 8 $\bar{9}$	4.25	2.97	2.61	2.13	0.80	1.60	1.23	1.56	0.999	0.753	0.862
887	2 $\bar{12}$ $\bar{1}$	$\bar{4}$ 9 $\bar{6}$	2 $\bar{1}$ 0	0 4 7	3.70	3.06	2.55	2.45	2.41	0.23	0.99	1.57	-0.999	0.752	0.863
888	7 0 5	$\bar{6}$ 2 3	0 1 $\bar{10}$	$\bar{1}$ $\bar{3}$ 2	4.25	3.00	2.77	2.11	0.96	0.48	0.88	1.66	-1.000	0.251	0.867
889	10 $\bar{8}$ $\bar{1}$	1 $\bar{1}$ 5	$\bar{6}$ 2 3	$\bar{5}$ 7 $\bar{7}$	3.80	3.39	3.00	2.51	0.85	1.23	0.41	2.15	0.999	0.253	0.870
890	2 7 $\bar{8}$	3 2 7	$\bar{4}$ $\bar{13}$ 0	$\bar{1}$ 4 1	4.17	3.10	2.40	2.32	2.05	0.32	1.39	1.61	0.999	0.745	0.871

Table 2. *Comparison of our* (3.13) *with Giacovazzo's* (13)

					Observed Magnitudes, |E|										
No.	$\vec{h}$	$\vec{k}$	$\vec{l}$	$\vec{m}$	$\vec{h}$	$\vec{k}$	$\vec{l}$	$\vec{m}$	$\vec{h}+\vec{k}$	$\vec{k}+\vec{l}$	$\vec{l}+\vec{m}$	B	COS(T)	P(+)	P(13)
566	4 $\bar{5}$ 7	$\bar{5}$ 6 $\bar{7}$	3 9 $\bar{1}$	$\bar{2}$ $\bar{10}$ 1	4.18	3.02	2.56	2.51	0.24	0.10	0.06	1.81	-1.000	0.029	0.017
570	4 $\bar{4}$ $\bar{8}$	$\bar{6}$ $\bar{1}$ 0	$\bar{5}$ 2 8	7 3 0	3.56	3.44	3.17	2.31	0.04	0.49	0.21	1.99	-1.000	0.030	0.019
593	9 1 $\bar{1}$	2 $\bar{12}$ $\bar{1}$	$\bar{8}$ 10 0	$\bar{3}$ 1 2	3.72	3.70	3.68	2.53	1.06	0.14	0.47	2.84	-1.000	0.033	0.124
663	7 0 5	2 7 8	9 $\bar{4}$ 1	0 $\bar{3}$ 2	4.25	4.17	2.70	2.34	1.07	0.20	0.59	2.48	-1.000	0.055	0.224
763	4 $\bar{5}$ 7	$\bar{8}$ 10 0	3 $\bar{11}$ $\bar{3}$	1 6 $\bar{4}$	4.18	3.68	2.42	2.33	1.20	0.46	0.00	1.93	-1.000	0.104	0.328
793	4 $\bar{4}$ $\bar{8}$	3 0 $\bar{1}$	$\bar{2}$ $\bar{7}$ 9	$\bar{5}$ 11 0	3.56	2.99	2.79	2.77	1.25	0.16	0.29	1.83	-1.000	0.142	0.346
798	2 7 $\bar{8}$	4 $\bar{9}$ 6	3 0 $\bar{1}$	$\bar{9}$ 2 3	4.17	3.06	2.99	2.36	0.75	0.61	0.74	2.00	-1.000	0.145	0.248
800	4 $\bar{4}$ $\bar{8}$	$\bar{10}$ 5 1	3 0 $\bar{1}$	3 $\bar{1}$ 8	3.56	3.26	2.99	2.60	0.42	0.27	1.25	2.00	-1.000	0.148	0.402
806	1 $\bar{1}$ 5	$\bar{3}$ $\bar{10}$ 6	0 1 $\bar{10}$	2 10 $\bar{1}$	3.39	3.16	2.77	2.51	0.55	0.11	1.00	1.65	-1.000	0.152	0.227
809	4 $\bar{5}$ 7	$\bar{6}$ $\bar{1}$ 0	7 $\bar{7}$ $\bar{8}$	$\bar{5}$ 13 1	4.18	3.44	3.12	2.16	1.39	0.03	0.68	2.15	-1.000	0.155	0.705
813	6 1 0	$\bar{1}$ 1 $\bar{5}$	0 $\bar{1}$ 10	$\bar{5}$ $\bar{1}$ $\bar{5}$	3.44	3.39	2.77	2.20	0.09	1.00	0.53	1.58	-1.000	0.161	0.228
814	2 $\bar{12}$ $\bar{1}$	5 0 6	4 8 $\bar{8}$	$\bar{11}$ 4 3	3.70	3.04	2.80	2.24	1.00	0.30	0.46	1.57	-1.000	0.161	0.233
816	7 0 5	1 $\bar{5}$ $\bar{7}$	1 3 $\bar{2}$	$\bar{9}$ 2 4	4.25	3.96	2.11	2.09	1.36	0.36	0.40	1.65	-1.000	0.164	0.559
817	8 $\bar{10}$ 0	2 7 $\bar{9}$	$\bar{7}$ 2 8	$\bar{3}$ 1 1	3.68	2.79	2.76	2.67	0.61	0.62	0.71	1.68	-1.000	0.165	0.206
819	1 $\bar{5}$ $\bar{7}$	$\bar{3}$ $\bar{6}$ 3	3 6 $\bar{4}$	$\bar{1}$ 5 8	3.96	2.95	2.64	2.34	0.06	0.36	1.18	1.60	-1.000	0.164	0.307
837	8 $\bar{10}$ 0	$\bar{4}$ 9 $\bar{6}$	$\bar{7}$ 2 8	3 $\bar{1}$ $\bar{2}$	3.68	3.06	2.76	2.53	0.06	1.06	0.71	1.75	-1.000	0.185	0.335
838	4 $\bar{4}$ $\bar{8}$	$\bar{6}$ $\bar{1}$ 0	$\bar{2}$ $\bar{1}$ 0	4 6 8	3.56	3.44	2.58	2.26	0.04	0.30	1.27	1.58	-1.000	0.188	0.378
840	4 $\bar{4}$ $\bar{8}$	5 $\bar{6}$ 7	2 $\bar{1}$ 0	$\bar{11}$ 11 1	3.56	3.02	2.55	2.54	1.08	0.59	0.14	1.55	-1.000	0.193	0.316
844	2 $\bar{12}$ $\bar{1}$	$\bar{2}$ 11 0	3 0 $\bar{1}$	$\bar{3}$ 1 2	3.70	3.46	2.99	2.53	0.02	0.47	1.55	2.15	-1.000	0.195	0.796
849	4 $\bar{5}$ 7	$\bar{3}$ 0 1	$\bar{2}$ 0 2	1 5 $\bar{10}$	4.18	2.99	2.55	2.54	0.04	1.20	0.68	1.80	-1.000	0.199	0.455
866	4 $\bar{4}$ $\bar{8}$	3 0 $\bar{1}$	$\bar{10}$ 1 7	3 3 2	3.56	2.99	2.75	2.44	1.25	0.54	0.05	1.59	-1.000	0.215	0.440
874	7 0 5	$\bar{10}$ 1 7	3 $\bar{4}$ $\bar{10}$	0 3 $\bar{2}$	4.25	2.75	2.57	2.34	0.15	0.38	1.39	1.56	-1.000	0.228	0.540
876	2 7 $\bar{8}$	2 $\bar{12}$ $\bar{1}$	$\bar{2}$ 0 2	$\bar{2}$ 5 7	4.17	3.70	2.55	2.18	0.57	0.70	1.07	1.90	1.000	0.230	0.480
882	4 $\bar{5}$ 7	6 $\bar{3}$ $\bar{9}$	$\bar{8}$ 7 2	$\bar{2}$ 1 0	4.18	2.77	2.59	2.55	1.52	0.25	0.36	1.70	-1.000	0.238	0.705
889	10 $\bar{8}$ $\bar{1}$	1 $\bar{1}$ 5	$\bar{6}$ 2 3	$\bar{5}$ 7 $\bar{7}$	3.80	3.39	3.00	2.51	0.85	1.23	0.41	2.15	1.000	0.253	0.708
892	7 $\bar{6}$ 7	$\bar{7}$ $\bar{1}$ $\bar{4}$	$\bar{3}$ $\bar{6}$ 3	3 13 $\bar{6}$	3.36	3.12	2.95	2.37	0.22	1.40	0.43	1.62	1.000	0.256	0.580
895	7 0 5	$\bar{1}$ $\bar{3}$ $\bar{8}$	3 6 $\bar{3}$	$\bar{9}$ $\bar{3}$ 6	4.25	3.05	2.95	2.22	1.58	0.26	0.58	1.88	-1.000	0.257	0.845
897	8 $\bar{10}$ 0	$\bar{3}$ $\bar{2}$ $\bar{7}$	$\bar{7}$ 9 0	2 3 7	3.68	3.10	2.63	2.41	0.44	1.39	0.24	1.61	-1.000	0.260	0.576
899	7 0 5	$\bar{2}$ $\bar{6}$ $\bar{7}$	$\bar{1}$ $\bar{6}$ 4	$\bar{4}$ 12 $\bar{2}$	4.25	3.33	2.33	2.32	0.87	0.03	1.22	1.70	-1.000	0.263	0.606
905	7 0 5	$\bar{3}$ $\bar{4}$ $\bar{7}$	$\bar{5}$ $\bar{2}$ 6	1 6 $\bar{4}$	4.25	3.00	2.35	2.33	0.01	1.56	0.27	1.55	-1.000	0.269	0.691
906	1 9 $\bar{7}$	2 $\bar{11}$ 0	$\bar{6}$ 3 9	3 $\bar{1}$ $\bar{2}$	3.54	3.46	2.77	2.53	0.28	0.45	1.55	1.91	-1.000	0.268	0.789
907	10 $\bar{8}$ $\bar{1}$	$\bar{1}$ 8 $\bar{7}$	$\bar{9}$ $\bar{4}$ 1	0 4 7	3.80	3.29	2.70	2.45	1.14	0.71	0.61	1.84	1.000	0.268	0.583
913	4 $\bar{5}$ 7	$\bar{5}$ 6 $\bar{7}$	$\bar{2}$ 0 2	3 $\bar{1}$ $\bar{2}$	4.18	3.02	2.55	2.53	0.24	1.39	0.68	1.80	-1.000	0.277	0.697
915	1 9 $\bar{7}$	$\bar{6}$ $\bar{1}$ 0	4 2 7	1 $\bar{10}$ 0	3.54	3.44	2.62	2.20	0.68	0.95	0.67	1.56	1.000	0.278	0.424
920	2 7 $\bar{8}$	3 0 $\bar{1}$	$\bar{9}$ $\bar{7}$ 4	4 0 5	4.17	2.99	2.70	2.09	0.74	0.23	1.33	1.56	-1.000	0.296	0.644
929	2 7 $\bar{8}$	4 $\bar{10}$ 5	3 1 0	$\bar{9}$ 2 3	4.17	2.78	2.61	2.36	1.58	0.61	0.05	1.58	1.000	0.318	0.799
932	6 $\bar{6}$ 7	4 $\bar{4}$ $\bar{8}$	$\bar{2}$ $\bar{1}$ 0	$\bar{8}$ 11 1	3.57	3.56	2.58	2.35	0.82	1.27	0.35	1.72	-1.000	0.319	0.672
934	1 12 0	1 $\bar{1}$ 5	$\bar{2}$ $\bar{14}$ $\bar{3}$	0 3 $\bar{2}$	3.66	3.39	2.45	2.34	1.32	0.87	0.23	1.58	-1.000	0.324	0.708
939	1 12 0	$\bar{7}$ $\bar{1}$ $\bar{4}$	1 $\bar{7}$ 7	5 $\bar{4}$ $\bar{3}$	3.66	3.12	3.04	2.03	0.58	0.39	1.50	1.57	-1.000	0.341	0.763
951	2 7 $\bar{8}$	$\bar{5}$ 2 8	$\bar{2}$ 1 0	5 $\bar{10}$ 0	4.17	3.17	2.55	2.28	0.94	1.40	0.14	1.71	1.000	0.368	0.814

It is noteworthy that, employing some 300–400 of the most reliably estimated values of the invariants listed in Table 1, unique values were obtained, with perfect accuracy, for 230 of the phases having $|E|$ values greater than 2. Thus this structure is solvable *via* estimated values of the four-phase structure invariants alone.

6. Concluding remarks

Conditional probability distributions of the four-phase structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$ in $P\bar{1}$, given, in the first instance only the four magnitudes (2.1) and, in the second instance, all seven magnitudes (2.1) and (2.2), have been found. The distributions lead to estimates for φ dependent on these magnitudes. The initial applications strongly suggest that the results secured here will find important application in the solution of complex crystal structures in $P\bar{1}$. It is suggested that the methods described here, themselves an extension of some recent work in $P1$, can be extended to treat structure invariants and seminvariants in general, and that the concept of 'neighborhood of a structure invariant', introduced in an earlier paper (Hauptman, 1975*b*) will play the central role in this development.

7. Comparison with a recent result of Giacovazzo (1975)

Just as this paper was being prepared for submission, a paper by Giacovazzo (1975) appeared covering material closely related to ours but employing a different probabilistic background and a different mathematical formalism. Hence a rare opportunity presented itself to compare the different approaches.

First, it should be emphasized that, in using the Klug formalism, Giacovazzo assumes implicitly that the reciprocal vectors $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$ are fixed and that atomic coordinates are the primitive random variables. This assumption contrasts sharply with the one made here which is that the crystal structure is fixed and the reciprocal vectors $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$ are the primitive random variables. Thus there are two kinds of probability distribution which are conceptually quite distinct (a point made many times previously, *e.g.* Hauptman, 1975*a*), and there is no reason to suppose that corresponding distributions will be identical. It therefore comes as no surprise that none of Giacovazzo's distributions (11)–(13) agrees with our (3.13). In particular, Giacovazzo's conclusion that 'When N is large enough, (11) tells us that the product $E_1E_2E_3E_7$ (our $E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{l}}E_{\mathbf{m}}$) is probably positive when $E_4^2+E_5^2+E_6^2-2>0$ (in our notation $E^2_{\mathbf{h}+\mathbf{k}}+E^2_{\mathbf{k}+\mathbf{l}}+E^2_{\mathbf{l}+\mathbf{h}}-2>0$), probably negative when $E_4^2+E_5^2+E_6^2<2$.' cannot possibly follow from our (3.13) which implies instead that whether $P_+>\frac{1}{2}$ or $P_+<\frac{1}{2}$ depends on whether an intricate interrelationship among all seven magnitudes (2.1) and (2.2) holds and not merely on a relationship among the three magnitudes (2.2) alone. Again, it should be stressed that it is our distribution which is the appropriate one for crystal-structure analysis [refer again to Hauptman (1975*a*)], since one is ordinarily given a fixed but unknown crystal structure, and structure-factor amplitudes are sampled from reciprocal space. Finally, we make no use of the Gram–Charlier expansion in our analysis, in contrast to Giacovazzo's work, but employ instead a mathematical formalism only recently secured (*e.g.* Hauptman, 1975*a*, *b*). With this background then, the comparison between Giacovazzo's result and ours is particularly illuminating.

Observe next that Giacovazzo's chief result, (11) and (12), requires knowledge not only of seven magnitudes but of the sign of $E_4E_5E_6$ (our $E_{\mathbf{h}+\mathbf{k}}E_{\mathbf{k}+\mathbf{l}}E_{\mathbf{l}+\mathbf{h}}$) as well, whereas our (3.13) depends only on the seven magnitudes (2.1) and (2.2). Thus comparison is possible only between our (3.13) and Giacovazzo's (13), the special case that

$$|E_{\mathbf{h}+\mathbf{k}}E_{\mathbf{k}+\mathbf{l}}E_{\mathbf{l}+\mathbf{h}}|\simeq 0\,, \qquad (7.1)$$

since in this case the sign of $E_{\mathbf{h}+\mathbf{k}}E_{\mathbf{k}+\mathbf{l}}E_{\mathbf{l}+\mathbf{h}}$ is irrelevant.

Table 2 displays a large and representative sample of 40 invariants from Table 1 for which (7.1) is approximately satisfied, so that comparison between our (3.13) and Giacovazzo's (13) is possible. The last two columns, headed $P(+)$ and $P(13)$, show the values of P_+ as calculated from our (3.13) and Giacovazzo's (13) respectively. Comparison of the entries in these two columns reveals significant differences, and comparison with the true cosine values, cos (T), is particularly illuminating.

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