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On the Theory and Estimation of the Cosine Invariants Cos $(\varphi_l+\varphi_m+\varphi_n+\varphi_p)$*

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For fixed $\mathbf{h}_1,\mathbf{h}_2,\mathbf{h}_3$, subject to $\mathbf{h}_1+\mathbf{h}_2+\mathbf{h}_3=0$, and uniformly distributed $\mathbf{k}$, the conditional joint probability distribution of the pair of phases $\varphi_{\mathbf{k}},\varphi_{\mathbf{h}_1+\mathbf{k}}$, given $|E_{-\mathbf{h}_3+\mathbf{k}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{h}_1+\mathbf{k}}|$ is found. If $\mathbf{l}+\mathbf{m}+\mathbf{n}+\mathbf{p}=0$, this distribution leads, *via* a suitable sampling technique, to estimates having probabilistic validity for the cosine invariant $\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ in terms of the seven magnitudes $|E_{\mathbf{l}}|,|E_{\mathbf{m}}|,|E_{\mathbf{n}}|,|E_{\mathbf{p}}|,|E_{\mathbf{l}+\mathbf{m}}|,|E_{\mathbf{l}+\mathbf{n}}|,|E_{\mathbf{l}+\mathbf{p}}|$.

Introduction

Explicit formulas for the cosine seminvariants $\cos\varphi$ and $\cos(\varphi_1+\varphi_2)$, having exact validity under certain conditions, are now known for a number of space groups, and the algebraic techniques for deriving similar formulas in most of the other space groups have been described (Hauptman & Karle, 1953; Weeks & Hauptman, 1970; Hauptman, 1972*a*,*b*). Both algebraic and probabilistic methods are available for estimating the value of the cosine invariant $\cos(\varphi_1+\varphi_2+\varphi_3)$, and it is known for example that the expected value of the latter is $I_1(A)/I_0(A)$ where I_0,I_1 are modified Bessel functions, $A=(2/N^{1/2})|E_1E_2E_3|$, and N is the number of atoms, assumed identical, in the unit cell. Thus the average value of $\cos(\varphi_1+\varphi_2+\varphi_3)$ is positive and tends to unity with increasing A; its reliability as an estimate of the value of the cosine also increases with increasing A. Motivated by the Harker–Kasper inequalities, Schenk and de Jong have recently made some semi-empirical observations and applications of cosine quartets $\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ of special type (Schenk & de Jong, 1973; Schenk, 1973*a*, *b*, 1974). The theory and estimation of the general cosine invariant, $\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$, subject to $|E_{\mathbf{l}+\mathbf{m}}|\simeq|E_{\mathbf{l}+\mathbf{n}}|\simeq|E_{\mathbf{l}+\mathbf{p}}|\simeq 0$, has also been worked out (Hauptman, 1973, 1974). In the present paper the probabilistic theory of the general cosine invariant $\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ subject to no restrictive conditions is initiated. The theory leads to an estimate for the value of the cosine which, in marked contrast to the estimate for $\cos(\varphi_1+\varphi_2+\varphi_3)$, may lie anywhere between -1 and $+1$. In particular, if $B=(2/N)|E_{\mathbf{l}}E_{\mathbf{m}}E_{\mathbf{n}}E_{\mathbf{p}}|$ is sufficiently large and $|E_{\mathbf{l}+\mathbf{m}}|$, $|E_{\mathbf{l}+\mathbf{n}}|$, $|E_{\mathbf{l}+\mathbf{p}}|$ are also large, then the estimate is positive and tends to unity with increasing $|E_{\mathbf{l}+\mathbf{m}}|$, $|E_{\mathbf{l}+\mathbf{n}}|$, $|E_{\mathbf{l}+\mathbf{p}}|$. If, on the other hand, $|E_{\mathbf{l}+\mathbf{m}}|\simeq|E_{\mathbf{l}+\mathbf{n}}|\simeq|E_{\mathbf{l}+\mathbf{p}}|\simeq 0$, then the estimate is negative and tends to -1 with increasing B. The latter result has been recently secured (Hauptman, 1974) so that both the methods and results described here may be regarded as generalizations of this earlier work. Since the values of the cosine invariants, in particular those which are small or negative, are of great significance in direct methods of phase determination, it is anticipated that the results obtained here will have important application in the further development of these procedures.

1·1. *Intuitive background**

Let $\mathbf{l},\mathbf{m},\mathbf{n},\mathbf{p}$, be fixed reciprocal vectors which satisfy

$$\mathbf{l}+\mathbf{m}+\mathbf{n}+\mathbf{p}=0\,, \tag{1.1}$$

and assume that $E_{\mathbf{l}}|,|E_{\mathbf{m}}|,|E_{\mathbf{n}}|$, $|E_{\mathbf{p}}|$ are large. Fix the origin by means of

$$\varphi_{\mathbf{l}}=\varphi_{\mathbf{m}}=\varphi_{\mathbf{n}}=0\,. \tag{1.2}$$

Suppose next that $|E_{\mathbf{l}+\mathbf{m}}|,|E_{\mathbf{m}+\mathbf{n}}|$ [$=|E_{\mathbf{l}+\mathbf{p}}|$ in view of (1.1)] and $|E_{\mathbf{n}+\mathbf{l}}|$ are also large. Then it is well known that, under these conditions,

$$\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{-\mathbf{l}-\mathbf{m}}\simeq 0\,, \tag{1.3}$$

$$\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{-\mathbf{m}-\mathbf{n}}\simeq 0\,, \tag{1.4}$$

$$\varphi_{\mathbf{n}}+\varphi_{\mathbf{l}}+\varphi_{-\mathbf{n}-\mathbf{l}}\simeq 0\,, \tag{1.5}$$

so that, in view of (1.2),

$$\varphi_{\mathbf{l}+\mathbf{m}}\simeq\varphi_{\mathbf{m}+\mathbf{n}}\simeq\varphi_{\mathbf{n}+\mathbf{l}}\simeq 0\,. \tag{1.6}$$

It follows similarly, from (1.1), (1.2), (1.6) and the assumed conditions, that

$$\varphi_{\mathbf{l}+\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}}\simeq\varphi_{\mathbf{p}}\simeq 0\,, \tag{1.7}$$

$$\varphi_{\mathbf{m}+\mathbf{n}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{p}}\simeq\varphi_{\mathbf{p}}\simeq 0\,, \tag{1.8}$$

$$\varphi_{\mathbf{n}+\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{p}}\simeq\varphi_{\mathbf{p}}\simeq 0\,. \tag{1.9}$$

In short, with the origin fixed by means of (1.2),

$$\varphi_{\mathbf{p}}\simeq 0 \tag{1.10}$$

or, from (1.2),

$$\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}}\simeq 0\,. \tag{1.11}$$

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However, from (1.1), it follows that the left side of (1.11) is a structure invariant so that its value is independent of the choice of origin. In summary then, if $|E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{n}}|, |E_{\mathbf{p}}|, |E_{\mathbf{l+m}}|, |E_{\mathbf{l+n}}|, |E_{\mathbf{l+p}}|$ are all large, the value of the cosine invariant $\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ is probably positive.

Clearly, however, the cosine invariants must occasionally be negative. In view of the previous argument, it is plausible to suppose that the cosine will be negative precisely in the circumstance that the hypotheses of the preceding paragraph are grossly violated, that is that each of $|E_{\mathbf{l+m}}|, |E_{\mathbf{l+n}}|, |E_{\mathbf{l+p}}|$ is small. While this argument is only heuristic and by no means a rigorous proof, it does serve to motivate the mathematical analysis which follows and throws some light on the more quantitative results given in the sequel.

2. For fixed $\mathbf{h}_1$ and $\mathbf{h}_3$, the joint conditional probability distribution of the pair, $\varphi_{\mathbf{k}}, \varphi_{\mathbf{h}_1+\mathbf{k}}$, given $|E_{-\mathbf{h}_3+\mathbf{k}}|, |E_{\mathbf{k}}|, |E_{\mathbf{h}_1+\mathbf{k}}|$

Suppose that a crystal structure in the space group $P1$ and consisting of N identical point atoms in the unit cell is fixed, and let $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3$ be fixed reciprocal vectors satisfying

$$\mathbf{h}_1+\mathbf{h}_2+\mathbf{h}_3=0 . \tag{2.1}$$

Introduce the usual abbreviations,

$$E_j=E_{\mathbf{h}_j}, |E_j|=|E_{\mathbf{h}_j}|, \varphi_j=\varphi_{\mathbf{h}_j}, \quad j=1,2,3 , \tag{2.2}$$

$$\varphi=\varphi_1+\varphi_2+\varphi_3 , \tag{2.3}$$

where φ_j is the phase of the normalized structure factor E_j. Suppose that the vector $\mathbf{k}$ is a random variable which is uniformly distributed over reciprocal space. Then $E_{-\mathbf{h}_3+\mathbf{k}}, E_{\mathbf{k}}, E_{\mathbf{h}_1+\mathbf{k}}$, as functions of the primitive random variable $\mathbf{k}$, are themselves random variables and the joint probability distribution, correct to terms of order $1/N$, of the respective magnitudes and phases $|E_{-\mathbf{h}_3+\mathbf{k}}|, |E_{\mathbf{k}}|, |E_{\mathbf{h}_1+\mathbf{k}}|, \varphi_{-\mathbf{h}_3+\mathbf{k}}, \varphi_{\mathbf{k}}, \varphi_{\mathbf{h}_1+\mathbf{k}}$ is known to be (Tsoucaris, 1970; Hauptman, 1971, 1972*b*)

$$\begin{aligned} P(R_1,R_2,R_3;\ \Phi_1,\Phi_2,\Phi_3) &\simeq \frac{R_1R_2R_3}{\pi^3\Delta} \\ &\times \exp\left\{-\frac{1}{\Delta}\left[R_1^2\left(1-\frac{|E_1|^2}{N}\right)+R_2^2\left(1-\frac{|E_2|^2}{N}\right)\right.\right. \\ &\left.\left.+R_3^2\left(1-\frac{|E_3|^2}{N}\right)\right]\right\} \\ &\times \exp\left\{\frac{2}{N^{1/2}\Delta}[R_1R_2|E_3|\cos(\Phi_1-\Phi_2+\varphi_3)\right. \\ &+R_2R_3|E_1|\cos(\Phi_2-\Phi_3+\varphi_1) \\ &\left.+R_3R_1|E_2|\cos(\Phi_3-\Phi_1+\varphi_2)]\right\} \\ &\times \exp\left\{-\frac{2}{N\Delta}[R_1R_2|E_1E_2|\cos(\Phi_1-\Phi_2-\varphi_1-\varphi_2)\right. \\ &+R_2R_3|E_2E_3|\cos(\Phi_2-\Phi_3-\varphi_2-\varphi_3) \\ &\left.+R_3R_1|E_3E_1|\cos(\Phi_3-\Phi_1-\varphi_3-\varphi_1)]\right\} \\ &\times\left\{1-\frac{1}{4N}(R_1^4+R_2^4+R_3^4+4R_1^2R_2^2+4R_2^2R_3^2\right. \\ &\left.+4R_3^2R_1^2-12R_1^2-12R_2^2-12R_3^2+18)\right\} , \end{aligned} \tag{2·4}$$

where

$$R_1\geq 0 , \quad R_2\geq 0 , \quad R_3\geq 0 , \tag{2.5}$$

$$\Delta=1-\frac{1}{N}(|E_1|^2+|E_2|^2+|E_3|^2)+\frac{2|E_1E_2E_3|}{N^{3/2}} \times \cos\varphi\geq 0 , \tag{2·6}$$

and φ is defined by (2.3).

The reader can readily verify, by consulting the references cited if necessary, that (2.4) is a well behaved probability distribution in that it is (essentially) non-negative for all values of the variables $R_1, R_2, R_3, \Phi_1, \Phi_2, \Phi_3$ and parameters E_1, E_2, E_3, and is suitably normalized.

Suppose next that R_1, R_2, R_3 are fixed non-negative numbers and that the vector $\mathbf{k}$ is a random variable which is now uniformly distributed over that region of reciprocal space for which

$$|E_{-\mathbf{h}_3+\mathbf{k}}|=R_1, \quad |E_{\mathbf{k}}|=R_2 , \quad |E_{\mathbf{h}_1+\mathbf{k}}|=R_3 . \tag{2.7}$$

Then the phases $\varphi_{\mathbf{k}}, \varphi_{\mathbf{h}_1+\mathbf{k}}$, as functions of the primitive random variable $\mathbf{k}$, are themselves random variables. Denote by $P(\Phi_2,\Phi_3|R_1,R_2,R_3)$ the joint conditional probability distribution of the pair $\varphi_{\mathbf{k}}, \varphi_{\mathbf{h}_1+\mathbf{k}}$, given (2.7). Then $P(\Phi_2,\Phi_3|R_1,R_2,R_3)$ is obtained from (2.4) by fixing R_1, R_2, R_3, integrating with respect to Φ_1 from 0 to 2π, and multiplying by a suitable normalizing constant. This integration has already been carried out in a different context [Hauptman, 1971, equation (6.6)]. Thus, correct to terms of order $1/N$,

$$\begin{aligned} &P(\Phi_2,\Phi_3|R_1,R_2,R_3) \\ &\simeq \frac{1}{K}\exp\left\{\frac{2}{\Delta N^{1/2}}R_2R_3|E_1|\cos(\Phi_2-\Phi_3+\varphi_1)\right. \\ &\left.-\frac{2}{\Delta N}R_2R_3|E_2E_3|\cos(\Phi_2-\Phi_3-\varphi_2-\varphi_3)\right\} \\ &\times I_0\left\{\frac{2R_1}{\Delta N^{1/2}}[R_2^2|E_3|^2+R_3^2|E_2|^2\right. \\ &\left.+2R_2R_3|E_2E_3|\cos(\Phi_2-\Phi_3-\varphi_2-\varphi_3)]^{1/2}\right\} , \end{aligned} \tag{2.8}$$

where I_0 is the modified Bessel function, K is a normalizing parameter to be determined, and R_1, R_2, R_3 are fixed, preassigned, non-negative numbers.

In order to evaluate K, one integrates (2.8) with respect to Φ_2 and Φ_3 between 0 and 2π and equates the result to unity. To this end the sum of the two cosines in the exponent of (2.8) is replaced by a single cosine by means of the trigonometric identity

$$\sum_{i=1}^{n} A_i \cos(\varphi+\alpha_i)=X\cos(\varphi+\xi), \qquad (2.9)$$

where

$$X=\Big(\sum_{i,j\ 1}^{n} A_iA_j\cos(\alpha_i-\alpha_j)\Big)^{1/2}, \qquad (2.10)$$

$$X\cos\xi=\sum_{i=1}^{n} A_i\cos\alpha_i, \qquad (2.11)$$

$$X\sin\xi=\sum_{i=1}^{n} A_i\sin\alpha_i. \qquad (2.12)$$

Also, with the use of the addition formula for Bessel functions (Watson, 1958, pp. 358, 361), (2.8) finally becomes simply

$$P(\Phi_2,\Phi_3|R_1,R_2,R_3) \simeq \frac{1}{K}\exp\left\{\frac{2R_2R_3X}{\Delta N^{1/2}}\cos(\Phi_2-\Phi_3+\xi)\right\} \times \sum_{\mu=-\infty}^{\infty} I\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times\cos\mu(\Phi_2-\Phi_3-\varphi_2-\varphi_3), \qquad (2.13)$$

where, from (2.10)–(2.12),

$$X=\left[|E_1|^2-\frac{2|E_1E_2E_3|}{N^{1/2}}\cos\varphi+\frac{|E_2E_3|^2}{N}\right]^{1/2}, \qquad (2.14)$$

$$X\cos\xi=|E_1|\cos\varphi_1-\frac{|E_2E_3|}{N^{1/2}}\cos(\varphi_2+\varphi_3), \qquad (2.15)$$

$$X\sin\xi=|E_1|\sin\varphi_1+\frac{|E_2E_3|}{N^{1/2}}\sin(\varphi_2+\varphi_3), \qquad (2.16)$$

and φ is given by (2.3), so that X and ξ are independent of Φ_2 and Φ_3. In view of

$$\cos\mu(\Phi_2-\Phi_3-\varphi_2-\varphi_3) =\cos\mu(\Phi_2-\Phi_3+\xi)\cos\mu(\varphi_2+\varphi_3+\xi) +\sin\mu(\Phi_2-\Phi_3+\xi)\sin\mu(\varphi_2+\varphi_3+\xi), \qquad (2.17)$$

and the integral formulas (Watson, 1958)

$$\frac{1}{2\pi}\int_0^{2\pi}\exp(z\cos\varphi)\cos\mu\varphi d\varphi=I_\mu(z), \qquad (2.18)$$

$$\int_0^{2\pi}\exp(z\cos\varphi)\sin\mu\varphi d\varphi=0, \qquad (2.19)$$

the integration of (2.13) with respect to Φ_2 is readily performed:

$$\int_{\Phi_3=0}^{2\pi}\int_{\Phi_2=0}^{2\pi} P(\Phi_2,\Phi_3|R_1,R_2,R_3)d\Phi_2d\Phi_3 \simeq\int_{\Phi_3=0}^{2\pi}\frac{2\pi}{K}\sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) \times I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right) \times\cos\mu(\varphi_2+\varphi_3+\xi)d\Phi_3, \qquad (2.20)$$

the integrand of which is independent of Φ_3. The second integration is therefore immediate and leads to the desired expression for K,

$$K\simeq4\pi^2\sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times I_\mu\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right)\cos\mu(\varphi_2+\varphi_3+\xi), \qquad (2.21)$$

where X and ξ are given by (2.14)–(2.16).

In order to exhibit the dependence of K on φ explicitly, one first shows by mathematical induction on μ, that

$$\exp\{i\mu(\varphi_2+\varphi_3+\xi)\}=\left(\frac{|E_1|\exp(i\varphi)-\frac{|E_2E_3|}{N^{1/2}}}{|E_1|\exp(-i\varphi)-\frac{|E_2E_3|}{N^{1/2}}}\right)^{\mu/2}, \quad \mu=0,\pm1,\pm2,\dots. \qquad (2.22)$$

Then, from (2.22) and (2.14),

$$\cos\mu(\varphi_2+\varphi_3+\xi)=\tfrac{1}{2}\exp\{i\mu(\varphi_2+\varphi_3+\xi)\} +\tfrac{1}{2}\exp\{-i\mu(\varphi_2+\varphi_3+\xi)\} =\frac{1}{2X^\mu}\left\{\left(|E_1|\exp(i\varphi)-\frac{|E_2E_3|}{N^{1/2}}\right)^\mu +\left(|E_1|\exp(-i\varphi)-\frac{|E_2E_3|}{N^{1/2}}\right)^\mu\right\}. \qquad (2.23)$$

Substitution of (2.23) into (2.21) yields

$$K\simeq2\pi^2\sum_{\mu=-\infty}^{\infty}\frac{1}{X^\mu} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times I_\mu\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right)\left\{\left(|E_1|\exp(i\varphi)-\frac{|E_2E_3|}{N^{1/2}}\right)^\mu + \left(|E_1|\exp(-i\varphi)-\frac{|E_2E_3|}{N^{1/2}}\right)^\mu\right\}, \qquad (2.24)$$

an expression for K in which the dependence on φ is clear.

Another expression for K, independent of X, is obtained by noting that $I_{-\mu}=I_\mu$ so that the cosine function in (2.21) may be replaced by the exponential function and K becomes

$$K \simeq 4\pi^2 \sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times I_\mu\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right) \times \left(\frac{|E_1|\exp(-i\varphi) - \frac{|E_2E_3|}{N^{1/2}}}{|E_1|\exp(i\varphi) - \frac{|E_2E_3|}{N^{1/2}}}\right)^{\mu/2} . \qquad (2.25)$$

Finally, employing again the addition formula for Bessel Functions, and noting that $I_\mu(-z) = (-1)^\mu I_\mu(z)$,

$$K \simeq 4\pi^2 \sum_{\substack{\mu,\nu \\ -\infty}}^{\infty} (-1)^{\mu+\nu} I_\mu\left(\frac{2R_1R_2|R_3|}{\Delta N^{1/2}}\right) \times I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) I_\nu\left(\frac{2R_2R_3|E_1|}{\Delta N^{1/2}}\right) \times I_{\mu+\nu}\left(\frac{2R_2R_3|E_2E_3|}{\Delta N}\right) \cos \nu\varphi , \qquad (2.26)$$

so that again the dependence of K on $\cos \varphi$ is clear.

3. The conditional expected value of $\cos t\,(\varphi_{\mathbf{k}} + \varphi_{-\mathbf{h}_1-\mathbf{k}} + \varphi_{-\mathbf{h}_2} + \varphi_{-\mathbf{h}_3})$, given $|E_{-\mathbf{h}_3+\mathbf{k}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{h}_1+\mathbf{k}}|$

In this section the conditional expected value of the cosine invariant $\cos t(\varphi_{\mathbf{k}} + \varphi_{-\mathbf{h}_1-\mathbf{k}} + \varphi_{-\mathbf{h}_2} + \varphi_{-\mathbf{h}_3})$ is derived. Although only the special case $t=1$ is important in the applications, the analysis is carried out for arbitrary integral t in order to permit an estimate for the variance, which depends also on the case $t=2$, to be obtained. The estimate for the variance is needed later (§6).

The conditional expected value of the random variable $\cos t(\varphi_{\mathbf{k}} + \varphi_{-\mathbf{h}_1-\mathbf{k}} + \varphi_{-\mathbf{h}_2} + \varphi_{-\mathbf{h}_3})$, given (2.7), is found from (2.13) by means of

$$\varepsilon\{\cos t(\varphi_{\mathbf{k}} + \varphi_{-\mathbf{h}_1-\mathbf{k}} + \varphi_{-\mathbf{h}_2} + \varphi_{-\mathbf{h}_3})|R_1, R_2, R_3\} = \varepsilon$$

$$\simeq \frac{1}{K}\int_{\Phi_2=0}^{2\pi}\int_{\Phi_3=0}^{2\pi} \cos t(\Phi_2 - \Phi_3 - \varphi_2 - \varphi_3) \times \exp\left\{\frac{2R_2R_3X}{\Delta N^{1/2}}\cos(\Phi_2 - \Phi_3 + \xi)\right\} \times \sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times \cos \mu(\Phi_2 - \Phi_3 - \varphi_2 - \varphi_3)\,\mathrm{d}\Phi_2\mathrm{d}\Phi_3 , \qquad (3.1)$$

where X, ξ and K are given by (2.14)–(2.16) and (2.24)–(2.26). Proceeding as in §2, one finds

$$\varepsilon \simeq \frac{1}{2K}\int_{\Phi_2=0}^{2\pi}\int_{\Phi_3=0}^{2\pi} \exp\left\{\frac{2R_2R_3X}{\Delta N^{1/2}}\cos(\Phi_2 - \Phi_3) + \xi\right\} \times \sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times [\cos(\mu+t)(\Phi_2 - \Phi_3 - \varphi_2 - \varphi_3) + \cos(\mu-t)(\Phi_2 - \Phi_3 - \varphi_2 - \varphi_3)]\mathrm{d}\Phi_2\mathrm{d}\Phi_3 , \qquad (3.2)$$

$$\varepsilon \simeq \frac{2\pi^2}{K}\sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times \left\{I_{\mu+t}\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right)\cos[(\mu+t)(\varphi_2 + \varphi_3 + \xi)] + I_{\mu-t}\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right)\cos[(\mu-t)(\varphi_2 + \varphi_3 + \xi)]\right\}, \qquad (3.3)$$

$$\varepsilon \simeq \frac{2\pi^2}{K}\sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times I_{\mu+t}\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right)\left\{\left[\frac{|E_1|\exp(-i\varphi) - \frac{|E_2E_3|}{N^{1/2}}}{|E_1|\exp(i\varphi) - \frac{|E_2E_3|}{N^{1/2}}}\right]^{\frac{\mu+t}{2}} + \left[\frac{|E_1|\exp(i\varphi) - \frac{|E_2E_3|}{N^{1/2}}}{|E_1|\exp(-i\varphi) - \frac{|E_2E_3|}{N^{1/2}}}\right]^{\frac{\mu+t}{2}}\right\} \qquad (3.4)$$

and finally

$$\varepsilon\{\cos t(\varphi_{\mathbf{k}} + \varphi_{-\mathbf{h}_1-\mathbf{k}} + \varphi_{-\mathbf{h}_2} + \varphi_{-\mathbf{h}_3})|R_1, R_2, R_3\} \simeq \frac{F_t}{F_0} , \qquad (3.5)$$

where

$$F_t = F_t(|E_1|, |E_2|, |E_3|;\ R_1, R_2, R_3;\ \varphi) = 2\pi^2 \sum_{\mu=-\infty}^{\infty} I_\mu\left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) I_\mu\left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) \times I_{\mu+t}\left(\frac{2R_2R_3X}{\Delta N^{1/2}}\right) \times \frac{1}{X^{\mu+t}}\left\{\left(|E_1|\exp(i\varphi) - \frac{|E_2E_3|}{N^{1/2}}\right)^{\mu+t} + \left(|E_1|\exp(-i\varphi) - \frac{|E_2E_3|}{N^{1/2}}\right)^{\mu+t}\right\}, \qquad (3.6)$$

so that, from (2.24),

$$K = F_0 . \qquad (3.7)$$

Again, as in the derivation of (2.26), F_t may also be written

$$F_t=4\pi^2 \sum_{\mu,\nu=-\infty}^{\infty} (-1)^{\mu+\nu+t} I_\mu \left(\frac{2R_1R_2|E_3|}{\Delta N^{1/2}}\right) \times I_\mu \left(\frac{2R_1R_3|E_2|}{\Delta N^{1/2}}\right) I_\nu \left(\frac{2R_2R_3|E_1|}{\Delta N^{1/2}}\right) \times I_{\mu+\nu+t} \left(\frac{2R_2R_3|E_2E_3|}{\Delta N}\right) \cos \nu\varphi\,. \tag{3.8}$$

The conditional expected value of the cosine invariant (3.5) has been derived from the conditional distribution (2.13) in the standard way. The analysis however is rather lengthy and not trivial. It would therefore be desirable, if possible, to bypass the distribution in order to arrive at the expected value. Although initial efforts to derive (3.5) in this way have not yet been successful, the derivation of (3.5) without using the distribution (2.13) would surely be a significant contribution.

4. Suitable sampling of reciprocal space leads to the first estimate for the cosine invariant, $\cos t\,(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$

Suppose that $\mathbf{l},\mathbf{m},\mathbf{n},\mathbf{p}$ are fixed reciprocal vectors which satisfy

$$\mathbf{l}+\mathbf{m}+\mathbf{n}+\mathbf{p}=0 \tag{4.1}$$

so that $\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}}$ is a structure invariant. Define reciprocal vectors $\mathbf{h}_1,\mathbf{h}_2,\mathbf{h}_3$ by means of

$$\mathbf{h}_1=-\mathbf{l}-\mathbf{m}\,,\quad \mathbf{h}_2=-\mathbf{n}\,,\quad \mathbf{h}_3=-\mathbf{p} \tag{4.2}$$

so that, in view of (4.1),

$$\mathbf{h}_1+\mathbf{h}_2+\mathbf{h}_3=0\,. \tag{4.3}$$

Choose a sample of size two from reciprocal space by means of

$$\mathbf{k}=\mathbf{l}\,,\quad \mathbf{k}=\mathbf{m}\,. \tag{4.4}$$

Then

$$\begin{aligned}&\mathbf{h}_1=-\mathbf{l}-\mathbf{m},\ \mathbf{h}_2=-\mathbf{n},\ \mathbf{h}_3=-\mathbf{p},\\ &-\mathbf{h}_3+\mathbf{k}=\mathbf{l}+\mathbf{p},\ \mathbf{k}=\mathbf{l},\ \mathbf{h}_1+\mathbf{k}=-\mathbf{m};\\ &\mathbf{h}_1=-\mathbf{l}-\mathbf{m},\ \mathbf{h}_2=-\mathbf{n},\ \mathbf{h}_3=-\mathbf{p},\\ &-\mathbf{h}_3+\mathbf{k}=\mathbf{m}+\mathbf{p},\ \mathbf{k}=\mathbf{m},\ \mathbf{h}_1+\mathbf{k}=-\mathbf{l}\end{aligned} \tag{4.5}$$

for the respective members (4.4) of the sample and, in view of (3.5), one obtains an estimate for the expected value of $\cos t(\varphi_{\mathbf{k}}-\varphi_{\mathbf{h}_1+\mathbf{k}}-\varphi_2-\varphi_3)$ by means of

$$\begin{aligned}&\varepsilon\{\cos t(\varphi_{\mathbf{k}}-\varphi_{\mathbf{h}_1+\mathbf{k}}-\varphi_2-\varphi_3)\}=\tfrac{1}{2}\cos t(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})\\ &+\tfrac{1}{2}\cos t(\varphi_{\mathbf{m}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})=\cos t(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})\\ &\simeq \left\langle \frac{F_t}{F_0} \right\rangle_2\end{aligned} \tag{4.6}$$

where F_t is defined by (3.6) or (3.8). The average in (4.6), in view of (4.5), is taken over the two sets of values

$$\begin{aligned}&|E_1|=|E_{\mathbf{l}+\mathbf{m}}|,|E_2|=|E_{\mathbf{n}}|,|E_3|=|E_{\mathbf{p}}|,\\ &R_1=|E_{\mathbf{l}+\mathbf{p}}|,R_2=|E_{\mathbf{l}}|,R_3=|E_{\mathbf{m}}|,\varphi=\varphi_{\mathbf{l}+\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}};\\ &|E_1|=|E_{\mathbf{l}+\mathbf{m}}|,|E_2|=|E_{\mathbf{n}}|,|E_3|=|E_{\mathbf{p}}|,R_1=|E_{\mathbf{m}+\mathbf{p}}|,\\ &R_2=|E_{\mathbf{m}}|,R_3=|E_{\mathbf{l}}|,\varphi=\varphi_{\mathbf{l}+\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}}\,.\end{aligned} \tag{4.7}$$

One obtains five other estimates for $\cos t(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ by choosing successively

$$\mathbf{h}_1=-\mathbf{l}-\mathbf{n}\,,\quad \mathbf{h}_2=-\mathbf{m}\,,\quad \mathbf{h}_3=-\mathbf{p}\,, \tag{4.8}$$

with sample

$$\mathbf{k}=\mathbf{l}\,,\quad \mathbf{k}=\mathbf{n}; \tag{4.9}$$

$$\mathbf{h}_1=-\mathbf{l}-\mathbf{p}\,,\quad \mathbf{h}_2=-\mathbf{m}\,,\quad \mathbf{h}_3=-\mathbf{n}\,, \tag{4.10}$$

with sample

$$\mathbf{k}=\mathbf{l}\,,\quad \mathbf{k}=\mathbf{p}; \tag{4.11}$$

$$\mathbf{h}_1=-\mathbf{m}-\mathbf{n}\,,\quad \mathbf{h}_2=-\mathbf{l}\,,\quad \mathbf{h}_3=-\mathbf{p} \tag{4.12}$$

with sample

$$\mathbf{k}=\mathbf{m}\,,\quad \mathbf{k}=\mathbf{n}; \tag{4.13}$$

$$\mathbf{h}_1=-\mathbf{m}-\mathbf{p}\,,\quad \mathbf{h}_2=-\mathbf{l}\,,\quad \mathbf{h}_3=-\mathbf{n}\,, \tag{4.14}$$

with sample

$$\mathbf{k}=\mathbf{m}\,,\quad \mathbf{k}=\mathbf{p}; \tag{4.15}$$

and finally

$$\mathbf{h}_1=-\mathbf{n}-\mathbf{p}\,,\quad \mathbf{h}_2=-\mathbf{l}\,,\quad \mathbf{h}_3=-\mathbf{m}\,, \tag{4.16}$$

with sample

$$\mathbf{k}=\mathbf{n}\,,\quad \mathbf{k}=\mathbf{p}\,. \tag{4.17}$$

Averaging the six expressions like (4.6), one obtains an estimate, based on an overall sample of size twelve, for $\cos t(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$,

$$\cos t(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})\simeq \left\langle \frac{F_t}{F_0} \right\rangle_{12}, \tag{4.18}$$

in which F_t is defined by (3.6) or (3.8) and the average in (4.18) is, in view of (4.5) and (4.8)–(4.17), taken over the twelve sets of values for $|E_1|,|E_2|,|E_3|,R_1,R_2,R_3$, $\varphi=\varphi_1+\varphi_2+\varphi_3$, Δ and X defined by Table 1, (2.6) and (2.14).

Table 1. *The twelve sets of values over which the sums in* (4.18), (5.5) *and* (6.1) *are taken*

	$\lvert E_1\rvert$	$\lvert E_2\rvert$	$\lvert E_3\rvert$	R_1	R_2	R_3	$\varphi=\varphi_1+\varphi_2+\varphi_3$
1	$\lvert E_{\mathbf{l}+\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\varphi_{\mathbf{l}+\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}}$
2	$\lvert E_{\mathbf{l}+\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\varphi_{\mathbf{l}+\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}}$
3	$\lvert E_{\mathbf{l}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\varphi_{\mathbf{l}+\mathbf{n}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{p}}$
4	$\lvert E_{\mathbf{l}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{n}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\varphi_{\mathbf{l}+\mathbf{n}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{p}}$
5	$\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{l}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\varphi_{\mathbf{l}+\mathbf{p}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$
6	$\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\varphi_{\mathbf{l}+\mathbf{p}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$
7	$\lvert E_{\mathbf{m}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\varphi_{\mathbf{m}+\mathbf{n}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{p}}$
8	$\lvert E_{\mathbf{m}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{n}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\varphi_{\mathbf{m}+\mathbf{n}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{p}}$
9	$\lvert E_{\mathbf{m}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{m}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\varphi_{\mathbf{m}+\mathbf{p}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{n}}$
10	$\lvert E_{\mathbf{m}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}+\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\varphi_{\mathbf{m}+\mathbf{p}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{n}}$
11	$\lvert E_{\mathbf{n}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}+\mathbf{m}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\varphi_{\mathbf{n}+\mathbf{p}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$
12	$\lvert E_{\mathbf{n}+\mathbf{p}}\rvert$	$\lvert E_{\mathbf{l}}\rvert$	$\lvert E_{\mathbf{m}}\rvert$	$\lvert E_{\mathbf{p}+\mathbf{m}}\rvert$	$\lvert E_{\mathbf{p}}\rvert$	$\lvert E_{\mathbf{n}}\rvert$	$\varphi_{\mathbf{n}+\mathbf{p}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}$

5. The second estimates for the cosine invariant, $\cos t(\varphi_l+\varphi_m+\varphi_n+\varphi_p)$, dependent on magnitudes only

Owing to the presence of the six unknown invariants φ on the right-hand side of (4.18), this equation is not useful as an estimate for $\cos t(\varphi_l+\varphi_m+\varphi_n+\varphi_p)$. Employing the abbreviation

$$T_\nu(z)=\frac{I_\nu(z)}{I_0(z)}, \tag{5.1}$$

a more useful estimate is obtained by replacing $\cos \nu\varphi$ and Δ by their expected values thus,

$$\begin{aligned}\bar{C}_\nu&=\bar{C}_\nu(|E_1|,|E_2|,|E_3|)=\varepsilon\{\cos \nu\varphi\}\\&=\varepsilon\{\cos \nu(\varphi_1+\varphi_2+\varphi_3)\}=\varepsilon\{\exp (i\varphi)\}\\&\simeq\tfrac{1}{3}\left\{T_\nu\left(\frac{2|E_1E_2E_3|}{N^{1/2}\left(1-\frac{|E_1|^2}{N}\right)}\right)\right.\\&+T_\nu\left(\frac{2|E_1E_2E_3|}{N^{1/2}\left(1-\frac{|E_2|^2}{N}\right)}\right)\\&\left.+T_\nu\left(\frac{2|E_1E_2E_3|}{N^{1/2}\left(1-\frac{|E_3|^2}{N}\right)}\right)\right\}\end{aligned} \tag{5·2}$$

$$\simeq T_\nu\left(\frac{2|E_1E_2E_3|}{N^{1/2}}\right), \quad \text{if } N \text{ is large}, \tag{5.3}$$

$$\begin{aligned}\bar{\Delta}&=\bar{\Delta}(|E_1|,|E_2|,|E_3|)\\&=\varepsilon(\Delta)=1-\frac{1}{N}(|E_1|^2+|E_2|^2+|E_3|^2)\\&+\frac{2|E_1E_2E_3|}{N^{3/2}}\bar{C}_1\,.\end{aligned} \tag{5.4}$$

Then, in view of (3.5)–(3.8), (4.18) is replaced by

$$\cos t(\varphi_l+\varphi_m+\varphi_n+\varphi_p)\simeq\left\langle\frac{D_t}{D_0}\right\rangle_{12} \tag{5.5}$$

in which the average is taken over the twelve sets of values of $|E_1|,|E_2|,|E_3|$; R_1,R_2,R_3 defined by Table 1 and

$$\begin{aligned}D_t&=D_t(|E_1|,|E_2|,|E_3|;\ R_1,R_2,R_3)\\&=4\pi^2\sum_{\mu=-\infty}^{\infty}Y^{\mu+t}I_\mu\left(\frac{2R_1R_2|E_3|}{\bar{\Delta}N^{1/2}}\right)I_\mu\left(\frac{2R_1R_3|E_2|}{\bar{\Delta}N^{1/2}}\right)\\&\times I_{\mu+t}\left(\frac{2R_2R_3\bar{X}}{\bar{\Delta}N^{1/2}}\right)\end{aligned} \tag{5.6}$$

or

$$\begin{aligned}D_t&=4\pi^2\sum_{\substack{\mu,\nu\\-\infty}}^{\infty}(-1)^{\mu+\nu+t}I_\mu\left(\frac{2R_1R_2|E_3|}{\bar{\Delta}N^{1/2}}\right)\\&\times I_\mu\left(\frac{2R_1R_3|E_2|}{\bar{\Delta}N^{1/2}}\right)\times I_\nu\left(\frac{2R_2R_3|E_1|}{\bar{\Delta}N^{1/2}}\right)\\&\times I_{\mu+\nu+t}\left(\frac{2R_2R_3|E_2E_3|}{\bar{\Delta}N}\right)\bar{C}_\nu\end{aligned} \tag{5.7}$$

where $\bar{C}_\nu$ and $\bar{\Delta}$ are defined by (5·1)–(5·4) and, in view of (2.14),

$$Y=\frac{1}{\bar{X}}\left(|E_1|\bar{C}_1-\frac{|E_2E_3|}{N^{1/2}}\right), \tag{5·8}$$

$$\bar{X}=\left[|E_1|^2-\frac{2|E_1E_2E_3|}{N^{1/2}}\bar{C}_1+\frac{|E_2E_3|^2}{N}\right]^{1/2}. \tag{5·9}$$

In the applications which have been made so far, (5.6) and (5.7) have led to two values for (5.5) which however have been essentially identical, as was naturally anticipated. Equation (5.6) is a rapidly converging simple infinite sum whereas (5.7) is a double series. In the actual calculations it has been found that the time required to compute (5.6) is less, by about an order of magnitude, than the time required to calculate (5.7). For this reason (5.6) is to be preferred in the applications. However, because of its greater symmetry, (5.7) may prove to be more useful in the further development of the theory.

Although the sample on which the estimate for the cosine invariant (5.5) is based is rather small (size twelve), it appears to be adequate to yield reliable estimates for those cosines which are large and positive and, except for a still unexplained positive scaling parameter, for those cosines which are negative. The estimate is not reliable only when it falls in the middle range (0·0 to 0·7) and this fact appears to be a consequence of the rather large associated variance in this case (§§7 and 8).

6. The third estimates for $\cos t(\varphi_l+\varphi_m+\varphi_n+\varphi_p)$, using a weighted average

Instead of (5.5) in which it has been assumed that all contributors to the sums have equal weights, one may employ

$$\cos t(\varphi_l+\varphi_m+\varphi_n+\varphi_p)\simeq\frac{\sum_{12}w_t\frac{D_t}{D_0}}{\sum_{12}w_t} \tag{6.1}$$

where D_t is again given by (5.6) or (5.7) and the weight w_t is defined to be the reciprocal of the variance:

$$\begin{aligned}\frac{1}{w_t}&=V_t(|E_1|,|E_2|,|E_3|;\ R_1,R_2,R_3;\ \varphi)\\&=\mathrm{Var}\{\cos t(\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h_1}-\mathbf{k}}+\varphi_{-\mathbf{h_2}}+\varphi_{-\mathbf{h_3}})\}\\&=\varepsilon\{\cos^2 t(\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h_1}-\mathbf{k}}+\varphi_{-\mathbf{h_2}}+\varphi_{-\mathbf{h_3}})\}\\&-[\varepsilon\{\cos t(\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h_1}-\mathbf{k}}+\varphi_{-\mathbf{h_2}}+\varphi_{-\mathbf{h_3}})\}]^2\\&\simeq\tfrac{1}{2}+\tfrac{1}{2}\varepsilon\{\cos 2t(\varphi_{\mathbf{k}}+\varphi_{-\mathbf{h_1}-\mathbf{k}}+\varphi_{-\mathbf{h_2}}+\varphi_{-\mathbf{h_3}})\}\\&-\frac{F_t^2}{F_0^2}\simeq\tfrac{1}{2}+\tfrac{1}{2}\frac{F_{2t}}{F_0}-\frac{F_t^2}{F_0^2}\end{aligned} \tag{6.2}$$

$$\simeq\tfrac{1}{2}+\tfrac{1}{2}\frac{D_{2t}}{D_0}-\frac{D_t^2}{D_0^2}, \tag{6.3}$$

so that w_t, as given by (6.3), depends only on $|E_1|$ $|E_2|, |E_3|$, R_1, R_2, R_3. As before, the sums in (6.1) are taken over the twelve sets of values of $|E_1|, |E_2|, |E_3|$, R_1, R_2, R_3 defined by Table 1.

7. The applications

An idealized structure consisting of $N=29$ identical point atoms in the space group $P1$ was constructed and normalized structure factors and cosine invariants calculated as shown in Tables 2–4. The structure was designed to simulate an actual crystal structure; in particular it exhibited a great deal of overlap in the Patterson function. As before, $\mathbf{l}, \mathbf{m}, \mathbf{n}, \mathbf{p}$ satisfy

$$\mathbf{l}+\mathbf{m}+\mathbf{n}+\mathbf{p}=0\,. \tag{7.1}$$

Comparisons between the true values of representative samples of cosines and those calculated by means of (5.5) and (5.6) are shown in Tables 2–4 and the errors briefly summarized in Table 5. The cosines calculated to be most positive are in good agreement with the true values as shown by Tables 2 and 5. Those cosines calculated to be negative correctly identify the cosines which are in fact negative, but Tables 3 and 5 show that

Table 2. 35 *cosines calculated to be most positive* $(>0{\cdot}90)$ *with* $2{\cdot}00 \le B < 2{\cdot}10$

Serial Number	$\mathbf{l}$ $\lvert E_{\mathbf{l}}\rvert$	$\mathbf{m}$ $\lvert E_{\mathbf{m}}\rvert$	$\mathbf{n}$ $\lvert E_{\mathbf{n}}\rvert$	$\mathbf{p}$ $\lvert E_{\mathbf{p}}\rvert$	$\mathbf{l}+\mathbf{m}$ $\lvert E_{\mathbf{l}+\mathbf{m}}\rvert$	$\mathbf{l}+\mathbf{n}$ $\lvert E_{\mathbf{l}+\mathbf{n}}\rvert$	$\mathbf{l}+\mathbf{p}$ $\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	B	$\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ True	Calc. (5.5)&(5.6)	$\Delta\cos = \cos_t - \cos_c$
1	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{4}\ 4\ \bar{4}$ 2.765	$2\ \bar{2}\ \bar{4}$ 2.142	$5\ 1\ 6$ 1.614	$\bar{7}\ 1\ \bar{2}$ 2.917	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$2\ \bar{2}\ 8$ 2.243	2.000	0.9840	0.9453	+0.0387
2	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{7}\ 1\ \bar{2}$ 2.917	$3\ \bar{4}\ \bar{4}$ 2.488	$7\ 6\ 4$ 1.325	$\bar{10}\ \bar{2}\ 0$ 1.987	$0\ \bar{7}\ \bar{2}$ 3.053	$4\ 3\ 6$ 2.924	2.012	0.9820	0.9409	+0.0411
3	$\bar{1}\ 2\ \bar{1}$ 2.862	$9\ \bar{1}\ \bar{1}$ 2.566	$1\ 5\ 3$ 2.073	$\bar{9}\ \bar{6}\ \bar{1}$ 1.958	$8\ 1\ \bar{2}$ 1.603	$0\ 7\ 2$ 3.053	$\bar{10}\ \bar{4}\ \bar{2}$ 2.525	2.056	0.9951	0.9267	+0.0684
4	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{6}\ 8\ \bar{1}$ 2.458	$9\ \bar{4}\ \bar{2}$ 2.176	$0\ \bar{1}\ 1$ 1.803	$\bar{9}\ 5\ 1$ 2.201	$6\ \bar{7}\ 0$ 2.626	$\bar{3}\ \bar{4}\ 3$ 2.275	2.018	0.7968	0.9266	−0.1298
5	$\bar{1}\ 2\ \bar{1}$ 2.862	$\bar{9}\ 1\ 1$ 2.566	$2\ 3\ 3$ 2.289	$8\ \bar{6}\ \bar{3}$ 1.802	$\bar{10}\ 3\ 0$ 2.201	$1\ 5\ 2$ 3.087	$7\ \bar{4}\ \bar{4}$ 1.183	2.089	0.7871	0.9258	−0.1387
6	$\bar{3}\ \bar{3}\ 2$ 3.034	$9\ \bar{4}\ \bar{2}$ 2.176	$5\ 0\ \bar{6}$ 2.152	$\bar{11}\ 7\ 6$ 2.127	$6\ \bar{7}\ 0$ 2.951	$2\ \bar{3}\ \bar{4}$ 2.830	$\bar{14}\ 4\ 8$ 1.606	2.084	0.9987	0.9254	+0.0733
7	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{4}\ 4\ \bar{4}$ 2.765	$\bar{1}\ 2\ 0$ 2.217	$5\ 1\ 6$ 1.614	$\bar{4}\ \bar{3}\ \bar{6}$ 2.924	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$5\ \bar{6}\ 4$ 1.085	2.083	0.9967	0.9225	+0.0742
8	$\bar{2}\ 3\ 4$ 2.830	$\bar{10}\ 4\ \bar{1}$ 2.454	$5\ 0\ \bar{6}$ 2.152	$7\ \bar{7}\ 3$ 2.023	$\bar{12}\ 7\ 3$ 1.850	$3\ 3\ \bar{2}$ 3.034	$5\ \bar{4}\ 7$ 2.039	2.085	0.8520	0.9214	−0.0694
9	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{7}\ 1\ \bar{2}$ 2.917	$\bar{1}\ \bar{1}\ \bar{2}$ 2.170	$11\ 3\ 2$ 1.538	$\bar{10}\ \bar{2}\ 0$ 1.987	$\bar{4}\ \bar{4}\ 0$ 2.242	$8\ 0\ 4$ 2.547	2.037	0.8717	0.9202	−0.0485
10	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{2}\ 3\ 4$ 2.830	$4\ 4\ 0$ 2.242	$\bar{2}\ 0\ \bar{2}$ 1.528	$\bar{2}\ \bar{4}\ 2$ 1.758	$4\ \bar{3}\ \bar{2}$ 2.015	$\bar{2}\ \bar{7}\ \bar{4}$ 3.109	2.041	0.9827	0.9195	+0.0632
11	$\bar{2}\ 3\ 4$ 2.830	$8\ \bar{1}\ \bar{3}$ 2.314	$5\ 0\ \bar{6}$ 2.152	$\bar{11}\ \bar{2}\ 5$ 2.071	$6\ 2\ 1$ 2.020	$3\ 3\ \bar{2}$ 3.034	$\bar{13}\ 1\ 9$ 1.824	2.013	0.7481	0.9188	−0.1707
12	$\bar{7}\ 1\ \bar{2}$ 2.917	$9\ \bar{4}\ \bar{2}$ 2.176	$\bar{1}\ \bar{1}\ \bar{2}$ 2.170	$\bar{1}\ 4\ 6$ 2.159	$2\ \bar{3}\ \bar{4}$ 2.830	$\bar{8}\ 0\ \bar{4}$ 2.547	$\bar{8}\ 5\ 4$ 1.441	2.051	0.9532	0.9185	+0.0347
13	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{3}\ \bar{3}\ 2$ 3.034	$5\ 1\ \bar{6}$ 2.158	$\bar{2}\ 9\ 6$ 1.491	$\bar{3}\ \bar{10}\ 0$ 1.989	$5\ \bar{6}\ \bar{8}$ 2.509	$\bar{2}\ 2\ 4$ 2.142	2.056	0.9902	0.9176	+0.0726
14	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{4}\ 4\ \bar{4}$ 2.765	$4\ 4\ 0$ 2.242	$0\ \bar{1}\ 6$ 1.571	$\bar{4}\ \bar{3}\ \bar{6}$ 2.924	$4\ \bar{3}\ \bar{2}$ 2.015	$0\ \bar{8}\ 4$ 1.795	2.051	0.9527	0.9168	+0.0359
15	$\bar{2}\ 3\ 4$ 2.830	$\bar{4}\ \bar{4}\ 0$ 2.242	$1\ 1\ 2$ 2.170	$5\ 0\ \bar{6}$ 2.152	$\bar{6}\ \bar{1}\ 4$ 1.559	$\bar{1}\ 4\ 6$ 2.159	$3\ 3\ \bar{2}$ 3.034	2.043	0.9842	0.9156	+0.0686
16	$\bar{5}\ \bar{2}\ 7$ 2.643	$\bar{6}\ 8\ \bar{1}$ 2.458	$9\ \bar{4}\ \bar{2}$ 2.176	$2\ \bar{2}\ \bar{4}$ 2.142	$\bar{11}\ 6\ 6$ 2.355	$4\ \bar{6}\ 5$ 1.936	$\bar{3}\ \bar{4}\ 3$ 2.275	2.088	0.9438	0.9154	+0.0284
17	$\bar{2}\ 3\ 4$ 2.830	$\bar{4}\ 4\ \bar{4}$ 2.765	$5\ 0\ \bar{6}$ 2.152	$1\ \bar{7}\ 6$ 1.725	$\bar{6}\ 7\ 0$ 2.626	$3\ 3\ \bar{2}$ 3.034	$\bar{1}\ \bar{4}\ 10$ 1.157	2.003	0.8132	0.9144	−0.1012
18	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$\bar{5}\ 10\ \bar{2}$ 2.303	$1\ \bar{2}\ 0$ 2.217	$5\ \bar{3}\ 4$ 1.868	$\bar{6}\ 5\ \bar{4}$ 1.426	$0\ \bar{7}\ \bar{2}$ 3.053	$4\ \bar{8}\ 2$ 2.183	2.031	0.9316	0.9133	+0.0183
19	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{3}\ 4\ 4$ 2.488	$2\ \bar{2}\ \bar{4}$ 2.142	$4\ 1\ \bar{2}$ 1.871	$\bar{6}\ 1\ 6$ 1.274	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$1\ \bar{2}\ 0$ 2.217	2.086	0.9744	0.9115	+0.0629
20	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{7}\ 1\ \bar{2}$ 2.917	$9\ \bar{5}\ \bar{1}$ 2.201	$1\ 7\ 1$ 1.524	$\bar{10}\ \bar{2}\ 0$ 1.987	$6\ \bar{8}\ 1$ 2.458	$\bar{2}\ 4\ 3$ 1.976	2.047	0.9473	0.9113	+0.0360
21	$\bar{10}\ 3\ 0$ 2.951	$1\ \bar{2}\ 1$ 2.862	$2\ \bar{3}\ \bar{4}$ 2.830	$7\ 2\ 3$ 1.220	$\bar{9}\ 1\ 1$ 2.566	$\bar{8}\ 0\ \bar{4}$ 2.547	$\bar{3}\ 5\ 3$ 1.490	2.011	0.9989	0.9111	+0.0878
22	$\bar{1}\ 2\ \bar{1}$ 2.862	$\bar{6}\ 7\ 0$ 2.626	$6\ 0\ 2$ 2.070	$1\ \bar{9}\ \bar{1}$ 1.887	$\bar{7}\ 9\ \bar{1}$ 1.446	$5\ 2\ 1$ 2.023	$0\ \bar{7}\ \bar{2}$ 3.053	2.025	0.9723	0.9084	+0.0639
23	$\bar{10}\ 3\ 0$ 2.951	$10\ \bar{4}\ 1$ 2.454	$1\ \bar{2}\ 0$ 2.217	$\bar{1}\ 3\ \bar{1}$ 1.864	$0\ \bar{1}\ 1$ 1.803	$\bar{9}\ 1\ 0$ 1.874	$\bar{11}\ 6\ \bar{1}$ 2.672	2.064	0.8137	0.9078	−0.0941
24	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$11\ \bar{6}\ 1$ 2.672	$\bar{4}\ 3\ \bar{5}$ 2.136	$\bar{6}\ 8\ 6$ 1.682	$10\ \bar{11}\ \bar{1}$ 2.290	$\bar{5}\ \bar{2}\ \bar{7}$ 1.799	$\bar{7}\ 3\ 4$ 2.207	2.044	0.8518	0.9077	−0.0559
25	$\bar{4}\ 4\ \bar{4}$ 2.765	$6\ \bar{7}\ 0$ 2.626	$\bar{6}\ 9\ \bar{1}$ 2.140	$4\ \bar{6}\ 5$ 1.936	$2\ \bar{3}\ \bar{4}$ 2.830	$\bar{10}\ 13\ \bar{5}$ 1.904	$0\ \bar{2}\ 1$ 1.643	2.075	0.9987	0.9071	+0.0916
26	$\bar{4}\ 4\ \bar{4}$ 2.765	$\bar{4}\ \bar{4}\ 0$ 2.242	$9\ \bar{4}\ \bar{2}$ 2.176	$\bar{1}\ 4\ 6$ 2.159	$\bar{8}\ 0\ \bar{4}$ 2.547	$5\ 0\ \bar{6}$ 2.152	$\bar{5}\ 8\ 2$ 1.658	2.008	0.9809	0.9070	+0.0739
27	$\bar{1}\ 2\ \bar{1}$ 2.862	$\bar{8}\ 1\ 3$ 2.314	$2\ \bar{4}\ 2$ 2.165	$7\ 1\ \bar{4}$ 2.108	$\bar{9}\ 3\ 2$ 2.092	$1\ \bar{2}\ 1$ 2.862	$6\ 3\ \bar{5}$ 1.436	2.084	0.8936	0.9070	−0.0136
28	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{2}\ 3\ 4$ 2.830	$9\ \bar{5}\ \bar{1}$ 2.201	$\bar{4}\ 5\ \bar{5}$ 1.540	$\bar{5}\ 0\ 6$ 2.152	$6\ \bar{8}\ 1$ 2.458	$\bar{7}\ 2\ \bar{3}$ 1.720	2.007	0.9976	0.9068	+0.0908
29	$\bar{3}\ \bar{3}\ 2$ 3.034	$5\ 1\ \bar{6}$ 2.158	$\bar{6}\ 9\ \bar{1}$ 2.140	$4\ \bar{7}\ 5$ 2.077	$2\ \bar{2}\ \bar{4}$ 2.142	$\bar{9}\ 6\ 1$ 1.454	$1\ \bar{10}\ 7$ 2.727	2.007	0.9471	0.9049	+0.0422
30	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{3}\ 4\ 4$ 2.488	$1\ \bar{2}\ 0$ 2.217	$2\ 5\ \bar{2}$ 1.726	$\bar{3}\ \bar{3}\ 2$ 3.034	$1\ \bar{9}\ \bar{2}$ 1.217	$2\ \bar{2}\ \bar{4}$ 2.142	2.005	0.8701	0.9032	−0.0331
31	$\bar{7}\ 1\ \bar{2}$ 2.917	$4\ \bar{4}\ 4$ 2.765	$\bar{4}\ \bar{4}\ 0$ 2.242	$7\ 7\ \bar{2}$ 1.631	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{11}\ \bar{3}\ \bar{2}$ 1.538	$0\ 8\ \bar{4}$ 1.795	2.034	0.9956	0.9030	+0.0926
32	$\bar{7}\ 1\ \bar{2}$ 2.917	$\bar{6}\ 8\ \bar{1}$ 2.458	$9\ \bar{3}\ \bar{2}$ 2.092	$4\ \bar{6}\ 5$ 1.936	$\bar{13}\ 9\ \bar{3}$ 2.176	$2\ \bar{2}\ \bar{4}$ 2.142	$\bar{3}\ \bar{5}\ 3$ 1.822	2.003	0.8684	0.9023	−0.0339
33	$\bar{10}\ 3\ 0$ 2.951	$6\ \bar{8}\ 1$ 2.458	$4\ 4\ 0$ 2.242	$0\ 1\ \bar{1}$ 1.803	$\bar{4}\ \bar{5}\ 1$ 1.160	$\bar{6}\ 7\ 0$ 2.626	$\bar{10}\ 4\ \bar{1}$ 2.454	2.022	0.8595	0.9020	−0.0425
34	$\bar{2}\ 3\ 4$ 2.830	$\bar{4}\ 4\ \bar{4}$ 2.765	$5\ 2\ 1$ 2.023	$1\ \bar{9}\ \bar{1}$ 1.887	$\bar{6}\ 7\ 0$ 2.626	$3\ 5\ 5$ 1.816	$\bar{1}\ \bar{6}\ 3$ 1.695	2.060	0.9768	0.9011	+0.0757
35	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{10}\ 3\ 0$ 2.951	$\bar{1}\ \bar{5}\ \bar{3}$ 2.073	$11\ 9\ 5$ 1.565	$\bar{10}\ \bar{4}\ \bar{2}$ 2.525	$\bar{1}\ \bar{12}\ \bar{5}$ 1.396	$11\ 2\ 3$ 2.251	2.016	0.9495	0.9008	+0.0487

Table 3. 33 *cosines calculated to be negative with* $0{\cdot}90 < B < 2{\cdot}16$

Serial Number	$\mathbf{l}$ $\lvert E_{\mathbf{l}}\rvert$	$\mathbf{m}$ $\lvert E_{\mathbf{m}}\rvert$	$\mathbf{n}$ $\lvert E_{\mathbf{n}}\rvert$	$\mathbf{p}$ $\lvert E_{\mathbf{p}}\rvert$	$\mathbf{l}+\mathbf{m}$ $\lvert E_{\mathbf{l}+\mathbf{m}}\rvert$	$\mathbf{l}+\mathbf{n}$ $\lvert E_{\mathbf{l}+\mathbf{n}}\rvert$	$\mathbf{l}+\mathbf{p}$ $\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	B	$\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ True	Calc. (5.5)&(5.6)	$\Delta\cos = \cos_t - \cos_c$
101	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$4\ 4\ 0$ 2.242	$4\ \bar{3}\ 5$ 2.136	$\bar{7}\ 4\ \bar{3}$ 2.014	$3\ \bar{1}\ \bar{2}$ 0.674	$3\ \bar{8}\ 3$ 0.282	$\bar{8}\ \bar{1}\ \bar{5}$ 0.922	2.053	−0.5070	−0.1428	−0.3642
102	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$1\ 1\ 2$ 2.170	$4\ \bar{3}\ 5$ 2.136	$\bar{4}\ 7\ \bar{5}$ 2.077	$0\ \bar{4}\ 0$ 0.385	$3\ \bar{8}\ 3$ 0.282	$\bar{5}\ 2\ \bar{7}$ 1.038	2.050	−0.6591	−0.2332	−0.4259
103	$\bar{1}\ 2\ \bar{1}$ 2.862	$11\ \bar{6}\ 1$ 2.672	$\bar{3}\ \bar{4}\ 3$ 2.275	$\bar{7}\ 8\ \bar{3}$ 1.700	$10\ \bar{4}\ 0$ 1.106	$\bar{4}\ \bar{2}\ 2$ 0.222	$\bar{8}\ 10\ \bar{4}$ 0.404	2.040	−0.9497	−0.2604	−0.6893
104	$\bar{8}\ 1\ 3$ 2.314	$1\ 8\ 1$ 1.973	$1\ \bar{3}\ 1$ 1.864	$6\ \bar{6}\ \bar{5}$ 1.576	$\bar{7}\ 9\ 4$ 0.661	$\bar{7}\ \bar{2}\ 4$ 0.111	$\bar{2}\ \bar{5}\ \bar{2}$ 0.253	0.925	−0.9990	−0.3508	−0.6482
105	$\bar{10}\ 4\ \bar{1}$ 2.454	$7\ \bar{4}\ 3$ 2.014	$7\ \bar{8}\ \bar{3}$ 1.591	$\bar{4}\ 8\ 1$ 1.870	$\bar{3}\ 0\ 2$ 0.398	$\bar{3}\ \bar{4}\ \bar{4}$ 0.177	$\bar{14}\ 12\ 0$ 0.612	1.015	−0.9817	−0.3528	−0.6289
106	$\bar{9}\ 1\ 1$ 2.566	$\bar{6}\ 8\ \bar{1}$ 2.458	$5\ \bar{2}\ \bar{2}$ 1.645	$10\ \bar{7}\ 2$ 1.555	$\bar{15}\ 9\ 0$ 0.875	$\bar{4}\ \bar{1}\ \bar{1}$ 0.166	$1\ \bar{6}\ 3$ 0.134	1.113	−0.8190	−0.3582	−0.4608
107	$\bar{9}\ 5\ 1$ 2.201	$7\ \bar{1}\ \bar{1}$ 1.957	$4\ 1\ \bar{2}$ 1.871	$\bar{2}\ \bar{5}\ 2$ 1.726	$\bar{2}\ 4\ 0$ 0.666	$\bar{5}\ 6\ \bar{1}$ 0.112	$\bar{11}\ 0\ 3$ 0.200	0.960	−0.9872	−0.3687	−0.6185
108	$1\ \bar{2}\ 1$ 2.862	$\bar{6}\ 10\ \bar{1}$ 1.934	$\bar{5}\ 2\ 2$ 1.645	$10\ \bar{10}\ \bar{2}$ 1.593	$\bar{5}\ 8\ 0$ 0.230	$\bar{4}\ 0\ 3$ 0.116	$11\ \bar{12}\ \bar{1}$ 0.698	1.001	−0.8904	−0.3727	−0.5177
109	$2\ \bar{3}\ \bar{4}$ 2.830	$9\ \bar{1}\ 0$ 1.874	$\bar{4}\ \bar{1}\ 1$ 1.731	$\bar{7}\ 5\ 3$ 1.654	$11\ \bar{4}\ \bar{4}$ 0.697	$\bar{2}\ \bar{4}\ \bar{3}$ 0.040	$\bar{5}\ 2\ \bar{1}$ 0.287	1.048	−0.9273	−0.3851	−0.5422
110	$\bar{4}\ 3\ 2$ 2.015	$\bar{9}\ 1\ 1$ 2.566	$3\ 3\ \bar{5}$ 2.001	$10\ \bar{7}\ 2$ 1.555	$\bar{13}\ 4\ 3$ 0.618	$\bar{1}\ 6\ \bar{3}$ 0.134	$6\ \bar{4}\ 4$ 0.374	1.110	−0.8465	−0.3990	−0.4475
111	$4\ \bar{3}\ \bar{5}$ 1.601	$10\ \bar{3}\ 0$ 2.951	$\bar{6}\ \bar{1}\ 2$ 1.588	$\bar{8}\ 7\ 3$ 1.798	$14\ \bar{6}\ \bar{5}$ 0.591	$\bar{2}\ \bar{4}\ \bar{3}$ 0.040	$\bar{4}\ 4\ \bar{2}$ 0.225	0.931	−0.7003	−0.4045	−0.2958
112	$\bar{5}\ \bar{2}\ 7$ 2.643	$\bar{3}\ \bar{5}\ 3$ 1.822	$2\ 6\ \bar{6}$ 1.763	$6\ 1\ \bar{4}$ 1.559	$\bar{8}\ \bar{7}\ 10$ 0.424	$\bar{3}\ 4\ 1$ 0.074	$1\ \bar{1}\ 3$ 0.387	0.913	+0.0169	−0.4063	+0.4232
113	$2\ \bar{5}\ 2$ 1.629	$3\ 3\ \bar{2}$ 3.034	$\bar{6}\ 4\ \bar{3}$ 1.604	$1\ \bar{2}\ 3$ 1.686	$5\ \bar{2}\ 0$ 0.543	$\bar{4}\ \bar{1}\ \bar{1}$ 0.166	$3\ \bar{7}\ 5$ 0.241	0.922	−0.8630	−0.4069	−0.4561
114	$0\ \bar{1}\ 1$ 1.803	$11\ \bar{6}\ 1$ 2.672	$\bar{4}\ \bar{1}\ 1$ 1.731	$\bar{7}\ 8\ \bar{3}$ 1.700	$11\ \bar{7}\ 2$ 0.414	$\bar{4}\ \bar{2}\ 2$ 0.223	$\bar{7}\ 7\ \bar{2}$ 0.399	0.978	−0.9851	−0.4104	−0.5747
115	$\bar{1}\ 2\ \bar{1}$ 2.862	$3\ \bar{2}\ \bar{5}$ 1.782	$\bar{3}\ \bar{4}\ 3$ 2.275	$1\ 4\ 3$ 1.513	$2\ 0\ \bar{6}$ 0.223	$\bar{4}\ \bar{2}\ 2$ 0.223	$0\ 6\ 2$ 0.710	1.212	−0.9750	−0.4113	−0.5637
116	$\bar{8}\ 1\ 3$ 2.314	$4\ \bar{3}\ \bar{2}$ 2.015	$1\ \bar{3}\ 1$ 1.864	$3\ 5\ \bar{2}$ 1.508	$\bar{4}\ \bar{2}\ 1$ 0.468	$\bar{7}\ \bar{2}\ 4$ 0.111	$\bar{5}\ 6\ 1$ 0.246	0.904	−0.9993	−0.4162	−0.5831
117	$\bar{9}\ 3\ 2$ 2.092	$2\ 5\ \bar{3}$ 2.216	$5\ \bar{3}\ 4$ 1.868	$2\ \bar{5}\ \bar{3}$ 1.633	$\bar{7}\ 8\ \bar{1}$ 0.513	$\bar{4}\ 0\ 6$ 0.121	$\bar{7}\ \bar{2}\ \bar{1}$ 0.283	0.976	−0.6636	−0.4184	−0.2452
118	$1\ \bar{2}\ 1$ 2.862	$\bar{2}\ 5\ 3$ 1.633	$\bar{5}\ 3\ \bar{4}$ 1.868	$6\ \bar{6}\ 0$ 1.517	$\bar{1}\ 3\ 4$ 0.120	$\bar{4}\ 1\ \bar{3}$ 0.221	$7\ \bar{8}\ 1$ 0.513	0.915	−0.4904	−0.4189	−0.0715
119	$\bar{10}\ 3\ 0$ 2.951	$\bar{1}\ 9\ 1$ 1.887	$8\ \bar{7}\ \bar{3}$ 1.798	$3\ \bar{5}\ 2$ 1.742	$\bar{11}\ 12\ 1$ 0.698	$\bar{2}\ \bar{4}\ \bar{3}$ 0.040	$\bar{7}\ \bar{2}\ 2$ 0.258	1.204	−0.7114	−0.4444	−0.2670
120	$\bar{1}\ 2\ \bar{1}$ 2.862	$\bar{6}\ 5\ 1$ 1.535	$\bar{3}\ \bar{4}\ 3$ 2.275	$10\ \bar{3}\ \bar{3}$ 1.518	$\bar{7}\ 7\ 0$ 0.414	$\bar{4}\ \bar{2}\ 2$ 0.223	$9\ \bar{1}\ \bar{4}$ 0.379	1.047	−0.9960	−0.4486	−0.5474
121	$0\ \bar{5}\ \bar{3}$ 2.193	$\bar{6}\ 9\ \bar{1}$ 2.140	$\bar{4}\ 3\ 5$ 1.601	$10\ \bar{7}\ \bar{1}$ 1.761	$\bar{6}\ 4\ \bar{4}$ 0.374	$\bar{4}\ \bar{2}\ 2$ 0.223	$10\ \bar{12}\ \bar{4}$ 0.104	0.913	−0.7748	−0.4508	−0.3240
122	$\bar{2}\ 4\ 3$ 1.976	$3\ 4\ \bar{3}$ 2.275	$0\ 0\ \bar{1}$ 1.875	$\bar{1}\ \bar{8}\ 1$ 1.631	$1\ 8\ 0$ 0.435	$\bar{2}\ 4\ 2$ 0.153	$\bar{3}\ \bar{4}\ 4$ 0.136	0.948	−0.9898	−0.4552	−0.5346
123	$\bar{6}\ 8\ \bar{1}$ 2.458	$7\ \bar{1}\ \bar{1}$ 1.957	$1\ \bar{2}\ 0$ 2.217	$\bar{2}\ \bar{5}\ 2$ 1.726	$1\ 7\ \bar{2}$ 0.698	$\bar{5}\ 6\ \bar{1}$ 0.112	$\bar{8}\ 3\ 1$ 0.190	1.269	−0.9332	−0.4600	−0.4732
124	$1\ 5\ 2$ 3.087	$\bar{4}\ 3\ \bar{5}$ 2.136	$\bar{6}\ \bar{1}\ 4$ 1.559	$9\ \bar{7}\ \bar{1}$ 1.572	$\bar{3}\ 8\ \bar{3}$ 0.282	$\bar{5}\ 4\ 6$ 0.094	$10\ \bar{2}\ 1$ 0.583	1.115	−0.6019	−0.4603	−0.1416
125	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{3}\ 0\ \bar{4}$ 1.893	$0\ 7\ \bar{1}$ 1.811	$6\ \bar{4}\ 3$ 1.604	$\bar{6}\ \bar{3}\ \bar{2}$ 0.530	$\bar{3}\ 4\ 1$ 0.074	$3\ \bar{7}\ 5$ 0.241	1.151	−0.9985	−0.5072	−0.4913
126	$\bar{5}\ 6\ \bar{6}$ 2.495	$4\ \bar{7}\ 5$ 2.077	$\bar{2}\ \bar{5}\ 2$ 1.726	$3\ 6\ \bar{1}$ 3.727	$\bar{1}\ \bar{1}\ \bar{1}$ 0.390	$\bar{7}\ 1\ \bar{4}$ 0.066	$\bar{2}\ 12\ \bar{7}$ 0.248	1.066	−0.9796	−0.5093	−0.4703
127	$1\ \bar{2}\ 0$ 2.217	$1\ \bar{2}\ 0$ 2.217	$\bar{9}\ 5\ 1$ 2.201	$7\ \bar{1}\ \bar{1}$ 1.957	$2\ \bar{4}\ 0$ 0.666	$\bar{8}\ 3\ 1$ 0.190	$8\ \bar{3}\ \bar{1}$ 0.190	1.460	−0.5405	−0.5126	−0.0279
128	$\bar{8}\ 7\ 0$ 2.152	$4\ \bar{3}\ \bar{2}$ 2.015	$7\ \bar{1}\ \bar{3}$ 1.814	$\bar{3}\ \bar{3}\ 5$ 2.001	$\bar{4}\ 4\ \bar{2}$ 0.225	$\bar{1}\ 6\ \bar{3}$ 0.134	$\bar{11}\ 4\ 5$ 0.349	1.086	−0.4919	−0.5219	+0.0300
129	$\bar{3}\ 4\ 4$ 2.488	$9\ \bar{1}\ \bar{1}$ 2.566	$\bar{7}\ 4\ \bar{3}$ 2.014	$1\ \bar{7}\ 0$ 1.565	$6\ 3\ 3$ 0.455	$\bar{10}\ 8\ 1$ 0.202	$\bar{2}\ \bar{3}\ 4$ 0.352	1.389	−0.8443	−0.5507	−0.2936
130	$4\ \bar{4}\ 4$ 2.765	$5\ 2\ \bar{7}$ 2.643	$\bar{7}\ 8\ \bar{3}$ 1.700	$\bar{2}\ \bar{6}\ 6$ 1.763	$9\ \bar{2}\ \bar{3}$ 0.154	$\bar{3}\ 4\ 1$ 0.074	$2\ \bar{10}\ 10$ 0.642	1.511	−0.6573	−0.5744	−0.0829
131	$1\ 5\ 2$ 3.087	$\bar{1}\ \bar{1}\ \bar{2}$ 2.170	$\bar{6}\ \bar{1}\ 4$ 1.559	$6\ \bar{3}\ \bar{4}$ 1.793	$0\ 4\ 0$ 0.385	$\bar{5}\ 4\ 6$ 0.094	$7\ 2\ \bar{2}$ 0.258	1.272	−0.7950	−0.6025	−0.1925
132	$2\ \bar{3}\ \bar{4}$ 2.830	$9\ \bar{1}\ \bar{1}$ 2.566	$\bar{3}\ \bar{3}\ 5$ 2.001	$\bar{8}\ 7\ 0$ 2.152	$11\ \bar{4}\ \bar{5}$ 0.349	$\bar{1}\ \bar{6}\ 1$ 0.176	$\bar{6}\ 4\ \bar{4}$ 0.374	2.158	−0.9853	−0.7376	−0.2477
133	$6\ \bar{7}\ 0$ 2.626	$9\ \bar{1}\ \bar{1}$ 2.566	$\bar{8}\ 7\ 0$ 2.152	$\bar{7}\ 1\ 1$ 1.957	$15\ \bar{8}\ \bar{1}$ 0.179	$\bar{2}\ 0\ 0$ 0.133	$\bar{1}\ \bar{6}\ 1$ 0.176	1.958	−0.9646	−0.7937	−0.1709

Table 4. 25 *cosines calculated in the middle range* $(0{\cdot}00$ *to* $+0{\cdot}70)$ *with* $2{\cdot}00 < B < 2{\cdot}10$

Serial Number	$\mathbf{l}$ $\lvert E_{\mathbf{l}}\rvert$	$\mathbf{m}$ $\lvert E_{\mathbf{m}}\rvert$	$\mathbf{n}$ $\lvert E_{\mathbf{n}}\rvert$	$\mathbf{p}$ $\lvert E_{\mathbf{p}}\rvert$	$\mathbf{l}+\mathbf{m}$ $\lvert E_{\mathbf{l}+\mathbf{m}}\rvert$	$\mathbf{l}+\mathbf{n}$ $\lvert E_{\mathbf{l}+\mathbf{n}}\rvert$	$\mathbf{l}+\mathbf{p}$ $\lvert E_{\mathbf{l}+\mathbf{p}}\rvert$	B	$\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ True	Calc. (5.5)&(5.6)	$\Delta\cos = \cos_t - \cos_c$
201	$0\ \bar{7}\ \bar{2}$ 3.053	$3\ \bar{4}\ \bar{4}$ 2.488	$\bar{9}\ 4\ 2$ 2.176	$6\ 7\ 4$ 1.777	$3\ \bar{11}\ \bar{6}$ 0.962	$\bar{9}\ \bar{3}\ 0$ 0.852	$6\ 0\ 2$ 2.070	2.026	0.9777	0.6936	+0.2841
202	$0\ \bar{7}\ \bar{2}$ 3.053	$5\ \bar{10}\ 2$ 2.303	$\bar{6}\ 9\ \bar{1}$ 2.140	$1\ 8\ 1$ 1.973	$5\ \bar{17}\ 0$ 1.519	$\bar{6}\ 2\ \bar{3}$ 1.113	$1\ 1\ \bar{1}$ 0.915	2.048	0.5872	0.6934	−0.1062
203	$\bar{3}\ \bar{3}\ 2$ 3.034	$\bar{6}\ 8\ \bar{1}$ 2.458	$1\ 1\ 2$ 2.170	$8\ \bar{6}\ \bar{3}$ 1.802	$\bar{9}\ 5\ 1$ 2.201	$\bar{2}\ \bar{2}\ 4$ 0.873	$5\ \bar{9}\ \bar{1}$ 0.877	2.011	−0.7546	0.6916	−1.4462
204	$\bar{3}\ \bar{3}\ 2$ 3.034	$7\ \bar{1}\ 2$ 2.917	$\bar{5}\ \bar{2}\ \bar{1}$ 2.023	$1\ 6\ \bar{3}$ 1.695	$4\ \bar{4}\ 4$ 2.765	$\bar{8}\ \bar{5}\ 1$ 0.819	$\bar{2}\ 3\ \bar{1}$ 0.775	2.093	0.9783	0.6892	+0.2891
205	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{1}\ 2\ 0$ 2.217	$\bar{6}\ 9\ \bar{1}$ 2.140	$7\ \bar{4}\ 3$ 2.014	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$\bar{6}\ 2\ \bar{3}$ 1.113	$7\ \bar{11}\ 1$ 0.500	2.013	0.9970	0.6873	+0.3097
206	$\bar{7}\ 1\ \bar{2}$ 2.917	$3\ 4\ \bar{3}$ 2.275	$\bar{1}\ \bar{1}\ \bar{2}$ 2.170	$5\ \bar{4}\ 7$ 2.039	$\bar{4}\ 5\ \bar{5}$ 1.540	$\bar{8}\ 0\ \bar{4}$ 2.547	$\bar{2}\ \bar{3}\ 5$ 0.247	2.025	0.2672	0.6838	−0.4166
207	$\bar{7}\ 1\ \bar{2}$ 2.917	$6\ \bar{7}\ 0$ 2.626	$7\ \bar{4}\ 3$ 2.015	$\bar{6}\ 10\ \bar{1}$ 1.934	$\bar{1}\ \bar{6}\ \bar{2}$ 1.406	$0\ \bar{3}\ 1$ 0.906	$\bar{13}\ 11\ \bar{3}$ 1.150	2.058	0.9995	0.6807	+0.3188
208	$\bar{3}\ \bar{3}\ 2$ 3.034	$9\ \bar{1}\ \bar{1}$ 2.566	$2\ \bar{2}\ \bar{4}$ 2.142	$\bar{8}\ 6\ 3$ 1.802	$6\ \bar{4}\ 1$ 0.522	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$\bar{11}\ 3\ 5$ 1.013	2.073	0.8149	0.6755	+0.1394
209	$\bar{1}\ 2\ \bar{1}$ 2.862	$6\ \bar{8}\ 1$ 2.458	$\bar{8}\ 1\ 3$ 2.314	$3\ 5\ \bar{3}$ 1.822	$5\ \bar{6}\ 0$ 1.169	$\bar{9}\ 3\ 2$ 2.092	$2\ 7\ \bar{4}$ 0.539	2.046	0.5524	0.6533	−0.1009
210	$\bar{7}\ 1\ \bar{2}$ 2.917	$\bar{1}\ 2\ \bar{1}$ 2.862	$5\ 2\ 1$ 2.023	$3\ \bar{5}\ 2$ 1.742	$\bar{8}\ 3\ \bar{3}$ 0.867	$\bar{2}\ 3\ \bar{1}$ 0.775	$\bar{4}\ \bar{4}\ 0$ 2.242	2.029	0.8685	0.6504	+0.2181
211	$\bar{10}\ 3\ 0$ 2.951	$3\ \bar{4}\ \bar{4}$ 2.488	$\bar{4}\ \bar{4}\ 0$ 2.242	$11\ 5\ 4$ 1.771	$\bar{7}\ \bar{1}\ \bar{4}$ 1.400	$\bar{14}\ \bar{1}\ 0$ 0.619	$1\ 8\ 4$ 1.358	2.010	0.3990	0.6344	−0.2354
212	$\bar{10}\ 3\ 0$ 2.951	$5\ 2\ \bar{6}$ 2.333	$2\ \bar{4}\ 2$ 2.165	$3\ \bar{1}\ 4$ 2.000	$\bar{5}\ 5\ \bar{6}$ 0.849	$\bar{8}\ \bar{1}\ 2$ 1.603	$\bar{7}\ 2\ 4$ 0.883	2.057	0.0611	0.6223	−0.5612
213	$\bar{2}\ 3\ 4$ 2.830	$6\ \bar{7}\ 0$ 2.626	$3\ 3\ \bar{5}$ 2.001	$\bar{7}\ 1\ 1$ 1.957	$4\ \bar{4}\ 4$ 2.765	$1\ 6\ \bar{1}$ 0.176	$\bar{9}\ 4\ 5$ 1.358	2.007	0.9055	0.6156	+0.2899
214	$\bar{1}\ 2\ \bar{1}$ 2.862	$\bar{11}\ 6\ \bar{1}$ 2.672	$6\ 2\ 1$ 2.020	$6\ \bar{10}\ 1$ 1.934	$\bar{12}\ 8\ \bar{2}$ 1.674	$5\ 4\ 0$ 1.744	$5\ \bar{8}\ 0$ 0.230	2.061	−0.2381	0.5953	−0.8334
215	$\bar{2}\ 3\ 4$ 2.830	$9\ \bar{1}\ \bar{1}$ 2.566	$1\ 5\ 3$ 2.073	$\bar{8}\ \bar{7}\ \bar{6}$ 1.999	$7\ 2\ 3$ 1.220	$\bar{1}\ 8\ 7$ 0.298	$\bar{10}\ \bar{4}\ \bar{2}$ 2.525	2.075	0.9507	0.5945	+0.3562
216	$\bar{2}\ 3\ 4$ 2.830	$9\ \bar{1}\ \bar{1}$ 2.566	$4\ 4\ 0$ 2.242	$\bar{11}\ \bar{6}\ \bar{3}$ 1.799	$7\ 2\ 3$ 1.220	$2\ 7\ 4$ 3.109	$\bar{13}\ \bar{3}\ 1$ 0.136	2.020	0.7187	0.5413	+0.1774
217	$0\ \bar{7}\ \bar{2}$ 3.053	$11\ \bar{6}\ 1$ 2.672	$\bar{4}\ 8\ \bar{2}$ 2.183	$\bar{7}\ 5\ 3$ 1.654	$11\ \bar{13}\ \bar{1}$ 1.011	$\bar{4}\ 1\ \bar{4}$ 0.681	$\bar{7}\ \bar{2}\ 1$ 1.332	2.032	0.2667	0.5310	−0.2643
218	$\bar{10}\ 3\ 0$ 2.951	$7\ \bar{1}\ 2$ 2.917	$\bar{5}\ \bar{2}\ \bar{1}$ 2.023	$8\ 0\ \bar{1}$ 1.733	$\bar{3}\ 2\ 2$ 1.146	$\bar{15}\ 1\ \bar{1}$ 1.024	$\bar{2}\ 3\ \bar{1}$ 0.775	2.081	−0.9214	0.5302	−1.4516
219	$\bar{2}\ 3\ 4$ 2.830	$\bar{6}\ 7\ 0$ 2.626	$\bar{2}\ \bar{3}\ \bar{3}$ 2.289	$10\ \bar{7}\ \bar{1}$ 1.761	$\bar{8}\ 10\ 4$ 2.248	$\bar{4}\ 0\ 1$ 0.755	$8\ \bar{4}\ 3$ 0.367	2.066	0.5127	0.4204	+0.0923
220	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$0\ \bar{7}\ \bar{2}$ 3.053	$\bar{9}\ 5\ 1$ 2.201	$10\ 7\ 3$ 1.443	$\bar{1}\ \bar{12}\ \bar{4}$ 1.132	$\bar{10}\ 0\ \bar{1}$ 0.824	$9\ 2\ 1$ 0.747	2.064	−0.1642	0.3921	−0.5563
221	$\bar{3}\ \bar{3}\ 2$ 3.034	$4\ \bar{4}\ 4$ 2.765	$5\ 2\ \bar{6}$ 2.333	$\bar{6}\ 5\ 0$ 1.485	$1\ \bar{7}\ 6$ 1.725	$2\ \bar{1}\ \bar{4}$ 0.606	$\bar{9}\ 2\ 2$ 0.606	2.004	0.7608	0.3745	+0.3863
222	$\bar{1}\ \bar{5}\ \bar{2}$ 3.087	$\bar{2}\ \bar{3}\ \bar{3}$ 2.289	$\bar{7}\ 3\ 4$ 2.207	$10\ 5\ 1$ 1.892	$\bar{3}\ \bar{8}\ \bar{5}$ 0.350	$\bar{8}\ \bar{2}\ 2$ 1.048	$9\ 0\ \bar{1}$ 1.300	2.035	−0.8689	0.3505	−1.2194
223	$0\ \bar{7}\ \bar{2}$ 3.053	$3\ 4\ \bar{3}$ 2.275	$\bar{2}\ \bar{5}\ 3$ 2.216	$\bar{1}\ 8\ 2$ 1.952	$3\ \bar{3}\ \bar{5}$ 1.181	$\bar{2}\ \bar{12}\ 1$ 0.774	$\bar{1}\ 1\ 0$ 0.396	2.072	−0.9987	0.1650	−1.1637
224	$0\ \bar{7}\ \bar{2}$ 3.053	$9\ \bar{1}\ \bar{1}$ 2.566	$1\ 1\ 2$ 2.170	$\bar{10}\ 7\ 1$ 1.761	$9\ \bar{8}\ \bar{3}$ 1.003	$1\ \bar{6}\ 0$ 0.344	$\bar{10}\ 0\ \bar{1}$ 0.824	2.065	−0.9109	0.0349	−0.9458
225	$\bar{7}\ 1\ \bar{2}$ 2.917	$\bar{1}\ 2\ \bar{1}$ 2.862	$\bar{3}\ \bar{4}\ 3$ 2.275	$11\ 1\ 0$ 1.552	$\bar{8}\ 3\ \bar{3}$ 0.867	$\bar{10}\ \bar{3}\ 1$ 1.114	$4\ 2\ \bar{2}$ 0.222	2.033	−0.9989	0.0164	−1.0153

Table 5. *Average error and average magnitude of the error in calculated cosines taken from Tables 2–4*

	Average error, $\langle \Delta \cos \rangle$	Average magnitude of the error, $\langle \lvert \Delta \cos \rvert \rangle$	Number of contributors to the average
From Table 2	+0·0129	0·0661	35
From Table 3	−0·3620	0·3894	33
From Table 4	−0·2982	0·5271	25

quantitative agreement is poor. Nevertheless, because the estimates tend to be consistently too large, *i.e.* not sufficiently negative, it is clear that rescaling the calculated values by an empirically determined numerical factor will bring the calculated values of these cosines into acceptable agreement with the true values. It is conjectured that the bias shown by Table 3 arises from the excessive overlap in the Patterson function which causes a larger number of extremely negative cosines to occur than predicted by the theory (which assumes no Patterson overlap). A measure of the degree of Patterson overlap is given by comparison of the values of the two parameters,

$$\langle (|E_{\mathbf{k}}|^2-1)^2 \rangle_{\mathbf{k}} \simeq 1.3\,, \quad \langle (|E_{\mathbf{k}}|^2-1)^3 \rangle_{\mathbf{k}} \simeq 4.6\,, \qquad (7.2)$$

with the theoretical values of 1 and 2 respectively when no overlap is present (Hauptman, 1964). Finally, Tables 4 and 5 show that those cosines calculated to be in the middle range (0·00 to +0·70) are in poor agreement with the true values, and it is not clear that the initially calculated values can be brought into acceptable agreement with the true values in any simple way. The poor agreement between calculated and true values for these cosines is undoubtedly a consequence, at least in part, of the relatively large associated variance.

8. Concluding remarks

In this paper the probabilistic theory of the cosine invariants $\cos(\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}+\varphi_{\mathbf{p}})$ has been initiated. The theory leads to estimates for these cosines in terms of the seven magnitudes $|E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{n}}|, |E_{\mathbf{p}}|, |E_{\mathbf{l}+\mathbf{m}}|, E|_{\mathbf{l}+\mathbf{n}}|$, $|E_{\mathbf{l}+\mathbf{p}}|$. On the basis of preliminary calculations it appears that the cosines calculated to be most positive serve effectively to identify those cosines which are in fact most positive, those calculated to be negative effectively identify the cosines which are in fact negative, but those calculated to be in the middle range (0·00 to 0·70) are not reliable indicators of the true values.

Further developments along the following lines are suggested: Derive improved distributions which take into account higher-order terms in $1/N$ and whatever overlap in the Patterson may be present. Derive conditional distributions of two phases from joint probability distributions of four or more structure factors in order to obtain estimates of the cosines dependent on more than seven magnitudes. It is anticipated that more accurate distributions, dependent as well on many magnitudes, will surely lead to improved estimates for the cosine invariants.

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