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Quintets: a Joint Probability Distribution of Fifteen Structure Factors

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It is assumed that a crystal structure in $P1$ is fixed and that the random variables (vectors) **h**, **k**, **l**, **m**, **n** are uniformly and independently distributed over the subset of reciprocal space defined by $\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=0$. Then the 15 structure factors $E_{\mathbf{h}}$, $E_{\mathbf{k}}$, $E_{\mathbf{l}}$, $E_{\mathbf{m}}$, $E_{\mathbf{n}}$, $E_{\mathbf{h}+\mathbf{k}}$, $E_{\mathbf{h}+\mathbf{l}}$, $E_{\mathbf{h}+\mathbf{m}}$, $E_{\mathbf{h}+\mathbf{n}}$, $E_{\mathbf{k}+\mathbf{l}}$, $E_{\mathbf{k}+\mathbf{m}}$, $E_{\mathbf{k}+\mathbf{n}}$, $E_{\mathbf{l}+\mathbf{m}}$, $E_{\mathbf{l}+\mathbf{n}}$, $E_{\mathbf{m}+\mathbf{n}}$, as functions of the primitive random variables **h**, **k**, **l**, **m**, **n**, are themselves random variables, and their joint probability distribution is found. This distribution plays the central role in the theory and estimation of the five-phase structure invariants $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$.

1. Introduction

In recent work (Hauptman 1975*a*, *b*) a new method in the probabilistic theory of the structure invariants was initiated [and later extended to include the unequal atom case, in particular to neutron diffraction (Hauptman, 1976)]. Of particular importance was the introduction of the neighborhood concept which plays the central role in this development. In the previous paper (Hauptman, 1977) a sequence of nested neighborhoods of the five-phase structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$ was obtained. In the present paper joint probability distributions of five and of fifteen structure factors, associated with the first and second neighborhoods, respectively, of φ are derived. In the following paper (Hauptman & Fortier, 1977) the related conditional probability distributions of φ are obtained. The methods used are the same as those described in the earlier work (Hauptman, 1975*a*,*b*, 1976) with which it is assumed that the reader is familiar, so that the present paper is greatly abbreviated. However, Appendix II, available from the authors as a technical report of the Medical Foundation of Buffalo, contains complete details of the derivation for the 15-structure-factor distribution. Improvements and simplifications in the mathematical techniques have made it possible to carry out the extremely lengthy calculations in a reasonable time.

2. Joint probability distribution of the five structure factors $E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{n}}$

Suppose that a crystal structure, consisting of N atoms (not necessarily identical) per unit cell in $P1$, is fixed. The fivefold Cartesian product $W\times W\times W\times W\times W$ of reciprocal space W consists of all ordered quintuples (**h**, **k**, **l**, **m**, **n**), where **h**, **k**, **l**, **m**, **n** are reciprocal vectors. Suppose that the ordered quintuple of reciprocal vectors (**h**, **k**, **l**, **m**, **n**) is a random variable (vector) which is uniformly distributed over the subset of $W\times W\times W\times W\times W$ defined by

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=0\,. \tag{2.1}$$

Then the five normalized structure factors,

$$E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{n}}\,, \tag{2.2}$$

as functions of the primitive random variables, **h**, **k**, **l**, **m**, **n**, are themselves random variables. Denote by

$$P_5=P(R_1,R_2,R_3,R_4,R_5;\ \Phi_1,\Phi_2,\Phi_3,\Phi_4,\Phi_5) \tag{2.3}$$

the joint probability distribution of the magnitudes, $|E_{\mathbf{h}}|$, $|E_{\mathbf{k}}|$, $|E_{\mathbf{l}}|$, $|E_{\mathbf{m}}|$, $|E_{\mathbf{n}}|$, and the phases, $\varphi_{\mathbf{h}}$, $\varphi_{\mathbf{k}}$, $\varphi_{\mathbf{l}}$, $\varphi_{\mathbf{m}}$, $\varphi_{\mathbf{n}}$, of the five structure factors (2.2). Then, following the methods referred to earlier, one readily finds, correct up to and including terms of order $1/N^{3/2}$,

$$\begin{aligned}P_5\simeq\frac{1}{\pi^5}R_1R_2R_3R_4R_5\exp\Big\{&-(R_1^2+R_2^2+R_3^2+R_4^2+R_5^2)\\&-\frac{\sigma_4}{4\sigma_2^2}[R_1^4+R_2^4+R_3^4+R_4^4+R_5^4\\&-4(R_1^2+R_2^2+R_3^2+R_4^2+R_5^2)+10]\\&+\frac{2\sigma_5}{\sigma_2^{5/2}}R_1R_2R_3R_4R_5\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4+\Phi_5)\Big\},\end{aligned} \tag{2.4}$$

where

$$\sigma_n=\sum_{j=1}^{N}f_j^n\,, \tag{2.5}$$

and f_j is the zero-angle atomic scattering factor for the atom labeled j. In the X-ray diffraction case the f_j are the atomic numbers Z_j and are therefore all positive; in the neutron diffraction case some of the f_j may be negative. (2.4) leads directly to the conditional probability distribution of the structure invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$, given the magnitudes of the five structure factors (2.2), as shown in the accompanying paper (Hauptman & Fortier, 1977).

3. Joint probability distribution of the 15 structure factors $E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{n}}; E_{\mathbf{h+k}}, E_{\mathbf{h+l}}, E_{\mathbf{h+m}}, E_{\mathbf{h+n}}, E_{\mathbf{k+l}}, E_{\mathbf{k+m}}, E_{\mathbf{k+n}}, E_{\mathbf{l+m}}, E_{\mathbf{l+n}}, E_{\mathbf{m+n}}$

Under the same assumptions as in § 2 the 15 normalized structure factors

$$E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}, E_{\mathbf{n}};$$
$$E_{\mathbf{h+k}}, E_{\mathbf{h+l}}, E_{\mathbf{h+m}}, E_{\mathbf{h+n}}, E_{\mathbf{k+l}},$$
$$E_{\mathbf{k+m}}, E_{\mathbf{k+n}}, E_{\mathbf{l+m}}, E_{\mathbf{l+n}}, E_{\mathbf{m+n}}, \qquad (3.1)$$

as functions of the primitive random variables **h**, **k**, **l**, **m**, **n**, are themselves random variables. Denote by

$$P_{15} = P(R_1, R_2, R_3, R_4, R_5, R_{12}, R_{13}, R_{14}, R_{15}, R_{23}, R_{24}, R_{25}, R_{34}, R_{35}, R_{45}; \Phi_1, \Phi_2, \Phi_3, \Phi_4, \Phi_5, \Phi_{12}, \Phi_{13}, \Phi_{14}, \Phi_{15}, \Phi_{23}, \Phi_{24}, \Phi_{25}, \Phi_{34}, \Phi_{35}, \Phi_{45}) \qquad (3.2)$$

the joint probability distribution of the magnitudes, $|E|$, and phases, φ, of the 15 structure factors (3.1). Following the methods referred to earlier (Hauptman, 1975*a*, *b*, 1976) and described at length in Appendix II, which is available from the authors, P_{15}, the major result of this paper, has been obtained and is shown in Appendix I correct up to and including terms of order $1/N^{3/2}$. Here, only those terms in P_{15} are given which are needed to derive the conditional distribution described in the accompanying paper (Hauptman & Fortier, 1977) correct up to and including terms of order $1/N^{3/2}$:

$$\begin{aligned}
P_{15} = {} & \frac{1}{\pi^{15}} R_1R_2R_3R_4R_5R_{12}R_{13}R_{14} \\
& \times R_{15}R_{23}R_{24}R_{25}R_{34}R_{35}R_{45} \\
& \times \exp\Big\{ -R_1^2-R_2^2-R_3^2-R_4^2-R_5^2-R_{12}^2-R_{13}^2 \\
& -R_{14}^2-R_{15}^2-R_{23}^2-R_{24}^2-R_{25}^2-R_{34}^2-R_{35}^2-R_{45}^2 \\
& + \frac{2\sigma_3}{\sigma_2^{3/2}} [R_1R_2R_{12}\cos(\Phi_1+\Phi_2-\Phi_{12}) \\
& + R_1R_3R_{13}\cos(\Phi_1+\Phi_3-\Phi_{13}) \\
& + R_1R_4R_{14}\cos(\Phi_1+\Phi_4-\Phi_{14}) \\
& + R_1R_5R_{15}\cos(\Phi_1+\Phi_5-\Phi_{15}) \\
& + R_2R_3R_{23}\cos(\Phi_2+\Phi_3-\Phi_{23}) \\
& + R_2R_4R_{24}\cos(\Phi_2+\Phi_4-\Phi_{24}) \\
& + R_2R_5R_{25}\cos(\Phi_2+\Phi_5-\Phi_{25}) \\
& + R_3R_4R_{34}\cos(\Phi_3+\Phi_4-\Phi_{34}) \\
& + R_3R_5R_{35}\cos(\Phi_3+\Phi_5-\Phi_{35}) \\
& + R_4R_5R_{45}\cos(\Phi_4+\Phi_5-\Phi_{45})] \\
& + \frac{2\sigma_3}{\sigma_2^{3/2}} [R_1R_{23}R_{45}\cos(\Phi_1+\Phi_{23}+\Phi_{45}) \\
& + R_1R_{24}R_{35}\cos(\Phi_1+\Phi_{24}+\Phi_{35}) \\
& + R_1R_{25}R_{34}\cos(\Phi_1+\Phi_{25}+\Phi_{34}) \\
& + R_2R_{13}R_{45}\cos(\Phi_2+\Phi_{13}+\Phi_{45}) \\
& + R_2R_{14}R_{35}\cos(\Phi_2+\Phi_{14}+\Phi_{35}) \\
& + R_2R_{15}R_{34}\cos(\Phi_2+\Phi_{15}+\Phi_{34}) \\
& + R_3R_{12}R_{45}\cos(\Phi_3+\Phi_{12}+\Phi_{45}) \\
& + R_3R_{14}R_{25}\cos(\Phi_3+\Phi_{14}+\Phi_{25}) \\
& + R_3R_{15}R_{24}\cos(\Phi_3+\Phi_{15}+\Phi_{24}) \\
& + R_4R_{12}R_{35}\cos(\Phi_4+\Phi_{12}+\Phi_{35}) \\
& + R_4R_{13}R_{25}\cos(\Phi_4+\Phi_{13}+\Phi_{25}) \\
& + R_4R_{15}R_{23}\cos(\Phi_4+\Phi_{15}+\Phi_{23}) \\
& + R_5R_{12}R_{34}\cos(\Phi_5+\Phi_{12}+\Phi_{34}) \\
& + R_5R_{13}R_{24}\cos(\Phi_5+\Phi_{13}+\Phi_{24}) \\
& + R_5R_{14}R_{23}\cos(\Phi_5+\Phi_{14}+\Phi_{23})] - 2\left(\frac{3\sigma_3^2-\sigma_2\sigma_4}{\sigma_2^3}\right) \\
& \times [R_1R_2R_3R_{45}\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_{45}) \\
& + R_1R_2R_4R_{35}\cos(\Phi_1+\Phi_2+\Phi_4+\Phi_{35}) \\
& + R_1R_2R_5R_{34}\cos(\Phi_1+\Phi_2+\Phi_5+\Phi_{34}) \\
& + R_1R_3R_4R_{25}\cos(\Phi_1+\Phi_3+\Phi_4+\Phi_{25}) \\
& + R_1R_3R_5R_{24}\cos(\Phi_1+\Phi_3+\Phi_5+\Phi_{24}) \\
& + R_1R_4R_5R_{23}\cos(\Phi_1+\Phi_4+\Phi_5+\Phi_{23}) \\
& + R_2R_3R_4R_{15}\cos(\Phi_2+\Phi_3+\Phi_4+\Phi_{15}) \\
& + R_2R_3R_5R_{14}\cos(\Phi_2+\Phi_3+\Phi_5+\Phi_{14}) \\
& + R_2R_4R_5R_{13}\cos(\Phi_2+\Phi_4+\Phi_5+\Phi_{13}) \\
& + R_3R_4R_5R_{12}\cos(\Phi_3+\Phi_4+\Phi_5+\Phi_{12})] \\
& + 2\left(\frac{15\sigma_3^3-10\sigma_2\sigma_3\sigma_4+\sigma_2^2\sigma_5}{\sigma_2^{9/2}}\right) R_1R_2R_3R_4R_5 \\
& \times \cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4+\Phi_5)\Big\} \left\{1+O\left(\frac{1}{N}\right)\right\}.
\end{aligned} \qquad (3.3)$$

With the use of standard techniques, (3.3) leads to the conditional probability distribution of the structure invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$, given the magnitudes of the 15 structure factors (3.1), as shown in the following paper (Hauptman & Fortier, 1977); and $O(1/N)$ in (3.3) consists of those terms of order $1/N$ or higher which make a contribution only to terms of order $1/N^2$ or higher in the final conditional distribution.

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APPENDIX I

$$P_{15}=\frac{R_1R_2R_3R_4R_5R_{12}R_{13}R_{14}R_{15}R_{23}R_{24}R_{25}R_{34}R_{35}R_{45}}{\pi^{15}}\exp-\left(R_1^2+R_2^2+\ldots+R_{45}^2\right)$$

$$\times\exp\left(-\frac{\sigma_3^2}{\sigma_2^3}[R_1^2R_2^2+R_1^2R_{12}^2+R_2^2R_{12}^2+\ldots+R_4^2R_5^2+R_4^2R_{45}^2+R_5^2R_{45}^2+R_1^2R_{23}^2+R_1^2R_{45}^2+R_{23}^2R_{45}^2+\ldots\right.$$

$$+R_5^2R_{14}^2+R_5^2R_{23}^2+R_{14}^2R_{23}^2-7(R_1^2+R_2^2+\ldots+R_5^2)-4(R_{12}^2+R_{13}^2+\ldots+R_{45}^2)+25]$$

$$-\frac{\sigma_4}{4\sigma_2^2}[(R_1^4-4R_1^2+2)+\ldots+(R_{45}^4-4R_{45}^2+2)]+R_1R_2R_{12}\cos(\Phi_1+\Phi_2-\Phi_{12})$$

$$\times\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}+\frac{\sigma_5}{\sigma_2^{5/2}}(6-R_1^2-R_2^2-R_{12}^2)+\frac{2\sigma_3\sigma_4}{\sigma_2^{7/2}}[9+R_1^2+R_2^2+R_{12}^2-3(R_3^2+R_4^2+R_5^2)\right.$$

$$-2(R_{13}^2+R_{14}^2+R_{15}^2+R_{23}^2+R_{24}^2+R_{25}^2)-3(R_{34}^2+R_{35}^2+R_{45}^2)]$$

$$+\frac{2\sigma_3^3}{\sigma_2^{9/2}}(-24+R_1^2+R_2^2-5(R_3^2+R_4^2+R_5^2)$$

$$\left.\left.+3(R_{13}^2+R_{14}^2+R_{15}^2+R_{23}^2+R_{24}^2+R_{25}^2)+6(R_{34}^2+R_{35}^2+R_{45}^2)]\right\}\right)+\ldots\ 9\text{ terms}$$

$$+R_1R_{23}R_{45}\cos(\Phi_1+\Phi_{23}+\Phi_{45})\left\{\frac{2\sigma_3}{\sigma_2^{3/2}}+\frac{\sigma_5}{\sigma_2^{5/2}}(6-R_1^2-R_{23}^2-R_{45}^2)\right.$$

$$+\frac{2\sigma_3\sigma_4}{\sigma_2^{7/2}}[6+R_1^2-3(R_2^2+R_3^2+R_4^2+R_5^2)-2(R_{12}^2+R_{13}^2+R_{14}^2+R_{15}^2)$$

$$-(R_{24}^2+R_{25}^2+R_{34}^2+R_{35}^2)+R_{23}^2+R_{45}^2]$$

$$+\frac{2\sigma_3^3}{\sigma_2^{9/2}}[-19+R_1^2+5(R_2^2+R_3^2+R_4^2+R_5^2)+3(R_{12}^2+R_{13}^2+R_{14}^2+R_{15}^2)$$

$$\left.+R_{23}^2+R_{24}^2+R_{25}^2+R_{34}^2+R_{35}^2+R_{45}^2]\right\}+\ldots\ 14\text{ terms}$$

$$+R_1R_2R_3R_{45}\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_{45})\left(\frac{2\sigma_4}{\sigma_2^2}-\frac{6\sigma_3^2}{\sigma_2^3}\right)+\ldots\ 9\text{ terms}$$

$$+R_1R_2R_{13}R_{23}\cos(\Phi_1+\Phi_{23}-\Phi_2-\Phi_{13})\left(\frac{2\sigma_4}{\sigma_2^2}-\frac{4\sigma_3^2}{\sigma_2^3}\right)+\ldots\ 29\text{ terms}$$

$$+R_1R_{12}R_{13}R_{45}\cos(\Phi_1-\Phi_{12}-\Phi_{13}-\Phi_{45})\left(\frac{2\sigma_4}{\sigma_2^2}-\frac{4\sigma_3^2}{\sigma_2^3}\right)+\ldots\ 29\text{ terms}$$

$$+R_{12}R_{34}R_{13}R_{24}\cos(\Phi_{12}+\Phi_{34}-\Phi_{13}-\Phi_{24})\left(\frac{2\sigma_4}{\sigma_2^2}-\frac{2\sigma_3^2}{\sigma_2^3}\right)+\ldots\ 14\text{ terms}$$

$$+R_1R_2R_3R_4R_5\cos(\Phi_1+\Phi_2+\Phi_3+\Phi_4+\Phi_5)\left(\frac{2\sigma_5}{\sigma_2^{5/2}}-\frac{20\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{30\sigma_3^3}{\sigma_2^{9/2}}\right)$$

$$+R_1R_2R_3R_{14}R_{15}\cos(\Phi_1-\Phi_2-\Phi_3-\Phi_{14}-\Phi_{15})\left(\frac{2\sigma_5}{\sigma_2^{5/2}}-\frac{14\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{16\sigma_3^3}{\sigma_2^{9/2}}\right)+\ldots\ 29\text{ terms}$$

$$+R_{12}R_{23}R_{45}R_{14}R_{35}\cos(\Phi_{12}+\Phi_{23}+\Phi_{45}+\Phi_{14}+\Phi_{35})\left(\frac{2\sigma_5}{\sigma_2^{5/2}}-\frac{10\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{10\sigma_3^3}{\sigma_2^{9/2}}\right)+\ldots 11\text{ terms}$$

$$+R_{12}R_{13}R_{23}R_{45}^2 \cos(\Phi_{12}+\Phi_{13}+\Phi_{23}+2\Phi_{45})\left(\frac{\sigma_5}{\sigma_2^{5/2}}-\frac{6\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{6\sigma_3^3}{\sigma_2^{9/2}}\right)+\ldots \text{ 9 terms}$$

$$+R_1R_2R_{34}R_{13}R_{24} \cos(\Phi_1+\Phi_2+\Phi_{34}-\Phi_{13}-\Phi_{24})\left(\frac{2\sigma_5}{\sigma_2^{5/2}}-\frac{12\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{12\sigma_3^3}{\sigma_2^{9/2}}\right)+\ldots \text{ 59 terms}$$

$$+R_1^2R_{12}R_{13}R_{23} \cos(2\Phi_1+\Phi_{23}-\Phi_{12}-\Phi_{13})\left(\frac{\sigma_5}{\sigma_2^{5/2}}-\frac{6\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{6\sigma_3^3}{\sigma_2^{9/2}}\right)+\ldots \text{ 29 terms}$$

$$+R_1R_{12}R_{13}R_{24}R_{25}\cos(\Phi_1+\Phi_{13}+\Phi_{24}+\Phi_{25}-\Phi_{12})\left(\frac{2\sigma_5}{\sigma_2^{5/2}}-\frac{10\sigma_3\sigma_4}{\sigma_2^{7/2}}+\frac{8\sigma_3^3}{\sigma_2^{9/2}}\right)+\ldots \text{ 59 terms.}$$

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Quintets: the Probabilistic Theory of the Structure Invariant $\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$*

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It is assumed that a crystal structure in $P1$ is fixed and that the 15 non-negative numbers $R_1, R_2, R_3, R_4, R_5; R_{12}, R_{13}, R_{14}, R_{15}, R_{23}, R_{24}, R_{25}, R_{34}, R_{35}, R_{45}$ are also specified. The random variables (vectors) **h**, **k**, **l**, **m**, **n** are assumed to be uniformly and independently distributed in the regions of reciprocal space defined by

$$|E_{\mathbf{h}}|=R_1, |E_{\mathbf{k}}|=R_2, |E_{\mathbf{l}}|=R_3, |E_{\mathbf{m}}|=R_4, |E_{\mathbf{n}}|=R_5; \quad (1)$$

$$|E_{\mathbf{h+k}}|=R_{12}, |E_{\mathbf{h+l}}|=R_{13}, |E_{\mathbf{h+m}}|=R_{14}, |E_{\mathbf{h+n}}|=R_{15}, |E_{\mathbf{k+l}}|=R_{23},$$
$$|E_{\mathbf{k+m}}|=R_{24}, |E_{\mathbf{k+n}}|=R_{25}, |E_{\mathbf{l+m}}|=R_{34}, |E_{\mathbf{l+n}}|=R_{35}, |E_{\mathbf{m+n}}|=R_{45}: \quad (2)$$

and

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

Then the structure invariant $\varphi=\varphi_{\mathbf{h}}+\varphi_{\mathbf{k}}+\varphi_{\mathbf{l}}+\varphi_{\mathbf{m}}+\varphi_{\mathbf{n}}$, as a function of the primitive random variables **h**, **k**, **l**, **m**, **n**, is itself a random variable, and its conditional probability distribution, given (1) and (2), is derived. The distribution leads to estimates for $\cos\varphi$ in terms of the 15 magnitudes (1) and (2).

1. The probabilistic background

Suppose that a crystal structure consisting of N atoms (not necessarily identical) per unit cell in $P1$ is fixed and that the 15 non-negative numbers $R_1, R_2, R_3, R_4, R_5; R_{12}, R_{13}, R_{14}, R_{15}, R_{23}, R_{24}, R_{25}, R_{34}, R_{35}, R_{45}$ are also specified. Define the fivefold Cartesian product $W\times W\times W\times W\times W$ of reciprocal space W to be the collection of all ordered quintuples (**h**, **k**, **l**, **m**, **n**) where **h**, **k**, **l**, **m**, **n** are reciprocal vectors. Suppose next that the ordered quintuple of reciprocal vectors (**h**, **k**, **l**, **m**, **n**) is a random variable which is uniformly distributed over the subset of $W\times W\times W\times W\times W$ defined by

$$|E_{\mathbf{h}}|=R_1, |E_{\mathbf{k}}|=R_2, |E_{\mathbf{l}}|=R_3, |E_{\mathbf{m}}|=R_4, |E_{\mathbf{n}}|=R_5; \quad (1.1)$$

$$|E_{\mathbf{h+k}}|=R_{12}, |E_{\mathbf{h+l}}|=R_{13}, |E_{\mathbf{h+m}}|=R_{14}, |E_{\mathbf{h+n}}|=R_{15},$$
$$|E_{\mathbf{k+l}}|=R_{23}, |E_{\mathbf{k+m}}|=R_{24}, |E_{\mathbf{k+n}}|=R_{25}, |E_{\mathbf{l+m}}|=R_{34},$$
$$|E_{\mathbf{l+n}}|=R_{35}, |E_{\mathbf{m+n}}|=R_{45}; \quad (1.2)$$

and

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}+\mathbf{n}=0\,. \quad (1.3)$$

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