maxima. This result is not surprising because low l terms contribute a substantial portion of the whole Patterson function (after omitting the $l=0$ term) under the conditions of the test. However, as discussed in the article, these very low-l terms can hinder the true solution from showing up. This is clearly shown in Fig. 8, where the terms $l=2, 4$ were omitted from the calculations. It is worth noticing that the two omitted terms contributed 86% of the Patterson squared norm.

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Measurability of Bijvoet Differences in Triclinic, Monoclinic and Orthorhombic Crystals. II

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Abstract

The probability that the Bijvoet ratio X for the observed reflections of a given crystal is greater than any particular value X_0 depends on space-group symmetry, the number of anomalous scatterers per asymmetric unit and the parameters k and σ_1^2. Numerical values for this probability are obtained as a function of X_0 for different values of k and σ_1^2 for the triclinic, monoclinic and orthorhombic crystals containing p ($=1, 2, 3$ or 4) anomalous scatterers per asymmetric unit. These results are provided in the form of compact tables; Fortran programs that are useful in computing this probability for any given situation are also provided.

1. Introduction

The success of the anomalous-scattering method of structure determination strongly depends on the measurability of Bijvoet differences. The measurability is defined as the probability of the event $\{(X \geq 0{\cdot}1) \cap (y_{\min} \geq 0{\cdot}3)\}$ (Velmurugan & Parthasarathy, 1984; VP, hereafter) where X is the Bijvoet ratio and $y_{\min}$ is the minimum value of the normalized structure-factor magnitudes for the reflection $\mathbf{H}$ and the inverse reflection $\bar{\mathbf{H}}$. Owing to the importance of the anomalous-scattering method, particularly due to the advent of synchrotron radiation as a source for diffraction studies, it would be useful to know *a priori*, in the case of a given crystal, the percentage of *observed* reflections for which the Bijvoet ratio X would be greater than any specific value X_0, say. This information can be obtained from the probability value for the event $\{(X \geq X_0) \cap (y_{\min} \geq 0{\cdot}3)\}$ ($= D$, say) and we shall denote this probability by $M(X_0, 0{\cdot}3)$. The values of $M(X_0, 0{\cdot}3)$ for the particular case of $X_0 = 0{\cdot}1$ were obtained in VP for the triclinic, monoclinic and orthorhombic crystals containing one or two heavy atoms per asymmetric unit for values of k (*i.e.* the ratio of the imaginary to the total real part of the atomic scattering factor of the anomalous scatterer) up to 0·6. Under a pronounced anomalous-scattering effect, k can have larger values for some of the heavy atoms. For example, the values

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of k for Pr and Sm calculated from the measured values of dispersion corrections for these atoms at wavelengths very close to their absorbtion edges (Templeton, Templeton & Phizackerley, 1980; Templeton, Templeton, Phizackerley & Hodgson, 1982) are found to be 0·868 and 0·859 respectively. Hence it would be useful to obtain values of $M(X_0, 0{\cdot}3)$ for values of k up to 0·9. In proteins containing several thousand atoms per asymmetric unit it would be advantageous to use more than one heavy atom per asymmetric unit not only to increase the measurability but also to tackle the phase problem more effectively. Hence it would be useful to obtain the values of $M(X_0, 0{\cdot}3)$ for the cases $p=3$ and 4 also. In this paper we shall therefore obtain the values of $M(X_0, 0{\cdot}3)$ in the form of convenient tables for different values of X_0, for values of k up to 0·9 and for the cases in which $p=1, 2, 3$ and 4. These tables are useful for computing, in the case of a given crystal, the percentage of reflections for which the Bijvoet ratio would be greater than any specified value X_0.

2. Theoretical considerations

In this paper we shall follow the notation of VP. In particular, we shall use σ_1^2 to denote the fractional contribution to local mean intensity from the group of anomalous scatterers relative to the whole structure. We shall present the results corresponding to the non-centrosymmetric space-group categories 1, 3, 5 and 6 belonging to the triclinic, monoclinic and orthorhombic systems [see p. 59 of Lipson & Cohran (1966) for details of the space-group categories]. Since the theoretical expressions needed for the evaluation of $M(X, 0{\cdot}3)$ are available in VP, we shall give only the final expression needed for computing the numerical tables in this paper.

The theoretical expression for $M(X_0, 0{\cdot}3)$ in the case of a non-centrosymmetric crystal containing n atoms in the asymmetric unit of which p atoms are anomalous scatterers (of the same type) and the remaining q $(=n-p)$ are normal scatterers of similar scattering power is known to be [see equation (42) of VP]

$$M(X_0, 0{\cdot}3) = \Pr(D) = \int_D \cdots \int 2y_Q \exp(-y_Q^2)\, d\tau \quad (1)$$

where $d\tau$ is a volume element in the $(3p+2)$-dimensional Cartesian $(y_Q, \psi_0, \theta_1', \phi_1', \psi_1', \ldots, \theta_p', \phi_p', \psi_p')$ space. Equation (1) is valid for the space-group categories 5 and 6. For crystals of space-group category 3, $d\tau$ is the volume element in the $(2p+2)$-dimensional $(y_Q, \psi_0, \theta_1', \phi_1', \ldots, \theta_p', \phi_p')$ space. For crystals of space-group category 1, $d\tau$ is the volume element in the $(p+2)$-dimensional $(y_Q, \psi_0, \theta_1', \ldots, \theta_p')$ space. Thus (1) involves $(p+2)$-fold, $(2p+2)$-fold, $(3p+2)$-fold and $(3p+2)$-fold integrals for the space-group categories 1, 3, 5 and 6 respectively. The theoretical expressions for X and $y_{\min}$ in terms of the random variables involved in (1) are given by [see equation (27) of VP]

$$X = C_1 E_p y_Q |\sin(2\pi\psi_0)| / [C_2 E_p^2 + \sigma_2^2 y_Q^2 + C_3 E_p y_Q \cos(2\pi\psi_0)] \quad (2)$$

$$y_{\min} = \{\min[a + b(\cos 2\pi\psi_0 + k \sin 2\pi\psi_0), a + b(\cos 2\pi\psi_0 - k \sin 2\pi\psi_0)]\}^{1/2} \quad (3)$$

where a and b are defined to be

$$a = C_4 E_p^2/(\varepsilon p) + C_5 y_Q^2, \quad b = C_6 E_p y_Q/(\varepsilon p)^{1/2}.$$

The quantities C_i, $i=1$ to 6, depend on k, σ_1^2 and p and these are defined in equations (29) and (35) of VP. E_p is defined to be [see equation (22) of VP]

$$E = \left\{ \left[\sum_{j=1}^{p} \xi_{pj}(\theta_j', \phi_j', \psi_j') \right]^2 + \left[\sum_{j=1}^{p} \eta_{pj}(\theta_j', \phi_j', \psi_j') \right]^2 \right\}^{1/2}. \quad (4)$$

3. Discussion

The multiple integrals in (1) for the various space-group categories are to be computed by the Monte Carlo method for different values of X_0, p, k and σ_1^2. The results obtained for the space-group categories 1, 3, 5 and 6 corresponding to $p=1$, 2, 3 and 4 are given in Tables 1 to 16.* These tables contain the values of $M(X_0, 0{\cdot}3)$ corresponding to $\sigma_1^2 = 0{\cdot}02$, 0·05, 0·10, 0·15, 0·20, 0·30, 0·40 and 0·50 and $k = 0{\cdot}05$, 0·10, 0·15, 0·20, 0·25, 0·30, 0·40, 0·60, 0·80 and 0·90. Tables 1–4 are for space-group category 1 and pertain to the cases $p=1$, 2, 3 and 4 respectively. Tables 5–8 are for space-group category 3 and pertain to the cases $p=1$, 2, 3 and 4 respectively. Tables 9–12 are for space-group category 5 and pertain to the cases $p=1$, 2, 3 and 4 respectively. Tables 13–16 are for space-group category 6 and pertain to the cases $p=1$, 2, 3 and 4 respectively.

The variation of $M(X_0, 0{\cdot}3)$ as a function of X_0 is shown in Fig. 1 for the space-group category 5 corresponding to the following typical situation: $p=1$, $\sigma_1^2 = 0{\cdot}10$ and $k = 0{\cdot}05$, 0·10, 0·15, 0·20, 0·25, 0·30, 0·40, 0·60, 0·80 and 0·90. The ordinate corresponding to $X_0 = 0$ for any curve represents the probability of the event $\{(X \geq 0) \cap (y_{\min}) \geq 0{\cdot}3)\}$ and this event is equivalent to the event $\{y_{\min} \geq 0{\cdot}3\}$ $(= D_0$, say) since all the reflections satisfy the trivial condition that $X \geq 0$. Though the probability for the event D_0 is a

* Tables 1 to 16 have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43890 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

function of k and σ_1^2, it is found to be insensitive to changes in k and σ_1^2. For example, the values of Pr (D_0) (corresponding to $k = 0{\cdot}05$) are found to be 0·907 and 0·902 when $\sigma_1^2 = 0{\cdot}05$ and 0·30 respectively and the values of Pr (D_0) (corresponding to $\sigma_1^2 = 0{\cdot}05$) are found to be 0·907 and 0·852 for $k = 0{\cdot}05$ and 0·90 respectively. It is seen from Fig. 1 that the curves for M fall steeply to zero when k is small. For larger values of k, the curves fall relatively slowly. Thus, while it is hardly possible to find any reflection having a Bijvoet ratio greater than 0·25 when $k = 0{\cdot}05$, more than 61% of reflections would have a Bijvoet ratio greater than 0·25 when $k = 0{\cdot}9$. Curves for other values of k, σ_1^2 and p and for other space-group categories exhibit similar trends and hence are not shown. Since M varies differently in the different regions of σ_1^2 and k, values of M are given in Tables 1-16 at convenient unequal intervals of X_0.

In connection with the theoretical evaluation of $M(X_0, 0{\cdot}3)$ for any given X_0 for a particular crystal, the following points may be noted. Since M is a function of k and σ_1^2 and since these are, in turn, functions of $(\sin\theta)/\lambda$, it follows that M will also be a function of $(\sin\theta)/\lambda$. Hence it is necessary to obtain an average value of M ($\langle M\rangle$, say) for the crystal. $\langle M\rangle$ for a particular crystal can be obtained from the local values of M by giving weights proportional to the relative number of reflections in the various ranges of $(\sin\theta)/\lambda$. It can easily be shown that

$$\langle M\rangle = (3/S_{\max}^3) \int_0^{S_{\max}} Ms^2\, ds, \qquad (5)$$

where s stands for $(\sin\theta)/\lambda$ and $S_{\max}$ is the maximum value of $(\sin\theta)/\lambda$ for the data. The value of $\langle M\rangle$ for any situation (*i.e.* for given crystal, radiation and data) is to be obtained by carrying out the integration in (5) numerically. The values of M needed for the numerical integration can be obtained from the appropriate table of values of M by interpolation.

Reasonably good values of $\langle M\rangle$ can be obtained by employing the following simpler procedure: (i) Obtain the mean values of k and σ_1^2 for the data. (ii) Use these mean values to compute the value of $\langle M\rangle$ from the appropriate deposited table by a two-dimensional interpolation method (Abramowitz & Stegun, 1965). Fortran programs for calculating the value of $\langle M(X_0, 0{\cdot}3)\rangle$ corresponding to any fixed X_0 for a given crystal by this method are also available as deposited material.*

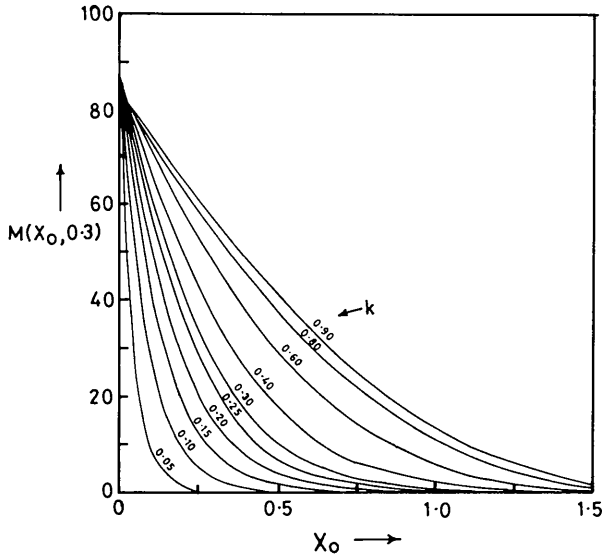

Fig. 1. Variation of $M(X_0, 0{\cdot}3)$ as a function of X_0 for the space-group category 5 corresponding to the situation in which $p = 1$ and $\sigma_1^2 = 0{\cdot}10$. The different curves correspond to the different values of k indicated.

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* See deposition footnote.

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