monoclinic binary axes in phase b is mainly controlled by long-range Coulomb interactions (Salje & Iishi, 1977) this is not true for the accompanying tilts of PO_4 groups. The critical temperature range (slow motion regime) is therefore larger than, for example, in $SrTiO_3$ (Müller & Berlinger, 1971). The correlation time of crystal field fluctuations was found to be greater than 10^{-8} s between 448 and 453 K (Razeghi & Houlier, 1978). Accordingly, phonon modes are overdamped in neutron scattering (Joffrin *et al.*, 1979) and infrared experiments (Luspin, Servoin & Gervais, 1979). Guimaraes (1979*b*) found highly anisotropic *B* factors in X-ray experiments, and the retarded splitting of Raman and infrared lines (Benoit, 1976) is probably also due to long-range fluctuations with extremely long relaxation times. From the given experimental results, the temperature range of the fluctuation regime is larger in $Pb_3(AsO_4)_2$ and some mixed crystals than in $Pb_3(PO_4)_2$. We therefore propose neutron scattering experiments, similar to those performed by Joffrin *et al.* (1979) on crystals with $x \gtrsim 0{\cdot}6$, where the thermal range of order-parameter fluctuations is enhanced compared with $Pb_3(PO_4)_2$.

Note added in proof: While this paper was in the press Dr Glazer informed us about the recent results of Wood, Wadhawan & Glazer (1981) concerning the temperature dependence of the optical birefringence of $Pb_3(PO_4)_2$. Their experimental results are in very good agreement with those shown in Fig. 10, $x = 0$. Their critical exponent $\beta = \frac{1}{4}$ for temperatures sufficiently below T_0 is identical with ours. It is noteworthy that the regime with $\beta = \frac{1}{2}$ near T_0 appears just for $Pb_3(PO_4)_2$ but not for all the quaternary oxides.

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The Effect of Data Truncation on the Measurability of Bijvoet Differences

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Abstract

Theoretical expressions for the complementary cumulative function of the Bijvoet ratio *X* applicable to a truncated data set are worked out for a non-centrosymmetric crystal containing *P* anomalous scatterers in the unit cell [$P = 1$ and many (*MN* and *MC* cases)] besides a large number of normal scatterers. These expressions contain the truncation limit y_t as a parameter of the distribution. The results obtained are

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used to discuss the effect of data truncation arising from the non-observability of extremely weak reflections on the measurability of Bijvoet differences.

1. Introduction

The earlier statistical studies on the normalized Bijvoet differences and the Bijvoet ratio were concerned with the influence of the structural features characterizing the crystal (*e.g.* the space-group symmetry, the number of anomalous scatterers per unit cell) on the measurability of Bijvoet differences (for a summary, see Srinivasan & Parthasarathy, 1976 – hereafter SP). It is clear that the measurability of Bijvoet differences will also be influenced by another important factor which is non-structural in origin but which is determined by the limitation of physical measurement itself. It is known that in any crystal not *all* theoretically possible reflections in a given $\sin\theta/\lambda$ range can actually be observed: there always exists a finite percentage of reflections whose intensities are too weak to be measured. Owing to the nonobservability of extremely weak reflections the observed data suffers a truncation (at the lower end).* It is relevant to ask how such a data truncation would affect the measurability of Bijvoet differences in a given crystal. A study of this problem is also interesting since larger Bijvoet ratios are generally believed to occur among extremely weak reflections (Ramachandran & Srinivasan, 1970). We shall therefore analyse this problem from a study of the theoretical complementary cumulative function (c.c.f. hereafter) of the Bijvoet ratio X† applicable to such truncated data. We shall consider three cases, namely the one-atom and many-atom ($P = MN$) and many-atom ($P = MC$) cases (for the notation and terminology see SP). In order to avoid theoretical complications, we shall restrict our studies to triclinic crystals of space group $P1$. However, the conclusions arrived at from the present study may be expected broadly to hold good in general.

The method of derivation of the c.c.f. of X is described in § 2. Since X is linearly related to another random variable v [see equation (2) for the definition of v] and since it is convenient to evaluate the c.c.f. of X from the c.c.f. of v, the c.c.f.'s of v for the various cases are derived in § 3. A discussion of the theoretical results is given in § 4. The probability formula required for the derivation of the truncated distribution from the untruncated distribution is derived in the Appendix.

* The truncated data consist of those reflections for which $y_N \geq y_t$ where y_t is the threshold value of the normalized structure amplitude y_N.

† This is denoted by δ in Parthasarathy & Parthasarathi (1973) (hereafter PP).

2. Method of derivation of the complementary cumulative function of X

Consider a non-centrosymmetric crystal containing N atoms in the unit cell of which P atoms are anomalous scatterers (of the same type) and the remaining $Q(= N - P)$ atoms are normal scatterers (of similar scattering power). The Bijvoet ratio X for the inverse reflections (hkl) and $(\bar{h}\bar{k}\bar{l})$ has been shown to be [see equations (2) and (5) of PP]

$$X = 4kv \tag{1}$$

where

$$v = \sigma_1 y_P \sin\theta_0 / y_N, \quad 0 \leq \theta_0 \leq \pi/2. \tag{2}$$

$P(v, y_N, \theta_0)$ [*i.e.* the joint probability density function (hereafter p.d.f.) of v, y_N and θ_0] for the one-atom and many-atom ($P = MC$) cases and $P(v, y_N)$ (*i.e.* the joint p.d.f. of v and y_N) for the many-atom ($P = MN$) case (valid for the untruncated data) are available in PP. From these functions and the result ($A4$) the joint p.d.f. applicable to the truncated data [*i.e.* $P_t(v, y_N, \theta_0)$ or $P_t(v, y_N)$] can be derived. The theoretical expression for the c.c.f. of v applicable to the truncated data [denoted by $N^c_{t,v}(v_0)$, where v_0 is a fixed value of v] can be derived from the truncated distribution function $P_t(v, y_N, \theta_0)$ [or $P_t(v, y_N)$] and this aspect is considered in § 3. Since $X = 4kv$ the c.c.f. of X valid for the truncated data [denoted by $N^c_{t,X}(X_0)$, where X_0 is a fixed value of X] can be obtained

$$\begin{aligned} N^c_{t,X}(X_0) &= N^c_{t,v}(X_0/4k) \\ &= 1 - N_{t,v}(X_0/4k). \end{aligned} \tag{3}$$

We shall therefore derive the c.c.f.'s* of v for the cases $P = 1$, MN and MC in § 3.

3. Derivation of the complementary cumulative function of v for the various cases

One-atom case

The joint p.d.f. of v, y_N and θ_0 (valid for the untruncated data) for this case has been shown to be [see equation (12) of PP]

$$\begin{aligned} P(v, y_N, \theta_0) = \frac{4y_N^2}{\pi\sigma_2^2 v} \exp\left[-\frac{y_N^2}{\sigma_2^2}\left(1 + \frac{v^2}{\sin^2\theta_0}\right)\right] \\ \times \cosh(2y_N^2 v \cot\theta_0/\sigma_2^2) \\ \times \delta(y_N - \sigma_1 \sin\theta_0/v), \\ 0 \leq y_N < \infty, \quad 0 \leq v < \infty, \quad 0 \leq \theta_0 \leq \pi/2. \end{aligned} \tag{4}$$

* In this paper we shall, for convenience, refer to the c.c.f. of v corresponding to the truncated data simply as the c.c.f. of v. We shall denote the cumulative function (hereafter c.f.) of v applicable to the truncated data by $N_{t,v}(v_0)$.

The joint p.d.f. of v, y_N and θ_0 applicable to the truncated data will therefore be given by [see (A4)]

$$P_t(v,y_N,\theta_0)=\frac{P(v,y_N,\theta_0)}{\beta_1}, \quad (5)$$

say, where β_1 is the value of the c.c.f. of y_N for $y_N=y_t$. From the p.d.f. of y_N for the one-atom case (SP) it follows that

$$\beta_1=1-\frac{2\exp(-\sigma_1^2/\sigma_2^2)}{\sigma_2^2}\times\int_0^{y_t} y_N\exp\left[-\frac{y_N^2}{\sigma_2^2}\right] I_0\left[\frac{2\sigma_1 y_N}{\sigma_2^2}\right]\mathrm{d}y_N. \quad (6)$$

It is convenient to use the simplifying notation

$$\sin\theta_0=S,\quad \cos\theta_0=C. \quad (7)$$

Substituting (4) in (5) and using the notation of (7) we obtain

$$P_t(v,y_N,\theta_0)=A(v,y_N,\theta_0)\,\delta\left(y_N-\frac{\sigma_1 S}{v}\right), \quad (8)$$

where $A(v,y_N,\theta_0)$ is defined to be

$$A(v,y_N,\theta_0)=\frac{4y_N^2}{\pi\sigma_2^2\beta_1 v}\exp\left[-\frac{y_N^2}{\sigma_2^2}\left(1+\frac{v^2}{S^2}\right)\right]\times\cosh\left[\frac{2y_N^2 vC}{\sigma_2^2 S}\right]. \quad (9)$$

The restriction on the range of v [see (8)] arises from the restriction of y_N to the interval y_t to ∞ and relation (2). The joint p.d.f. of v and θ_0 valid for the truncated data can be obtained from (8) as

$$P_t(v,\theta_0)=\int_{y_t}^{\infty}P_t(v,y_N,\theta_0)\,\mathrm{d}y_N$$

$$=\int_{y_t}^{\infty}A(v,y_N,\theta_0)\,\delta\left(y_N-\frac{\sigma_1 S}{v}\right)\mathrm{d}y_N. \quad (10)$$

Making use of the well known property of the Dirac delta function in (10) we obtain

$$P_t(v,\theta_0)=A\left(v,\frac{\sigma_1 S}{v},\theta_0\right)\quad \text{if}\ \frac{\sigma_1 S}{v}\geq y_t \quad (11)$$
$$=0\ \text{otherwise}.$$

Making use of (9) in (11) we obtain

$$P_t(v,\theta_0)=\frac{4\sigma_1^2 S^2}{\pi\sigma_2^2\beta_1 v^3}\exp\left[-\frac{\sigma_1^2}{\sigma_2^2}\left(1+\frac{S^2}{v^2}\right)\right]\times\cosh\left[\frac{2\sigma_1^2 CS}{\sigma_2^2 v}\right]. \quad (12)$$

The joint p.d.f. in (12) is non-zero only in the region defined by

$$\sin^{-1}\left(\frac{vy_t}{\sigma_1}\right)\leq\theta_0\leq\pi/2,\quad 0\leq v\leq\frac{\sigma_1}{y_t}. \quad (13)$$

The p.d.f. of v valid for the truncated data can be obtained from (12) as

$$P_t(v)=\frac{4\sigma_1^2 e^{-\sigma_1^2/\sigma_2^2}}{\pi\sigma_2^2\beta_1 v^3}\int_{\sin^{-1}(vy_t/\sigma_1)}^{\pi/2}S^2\exp-\frac{\sigma_1^2 S^2}{\sigma_2^2 v^2}\times\cosh\left[\frac{2\sigma_1^2 CS}{\sigma_2^2 v}\right]\mathrm{d}\theta_0. \quad (14)$$

The c.c.f. of v will therefore be given by

$$N_{t,v}^c(v_0)=\int_{v_0}^{\sigma_1/y_t}P_t(v)\,\mathrm{d}v=\frac{4\sigma_1^2 e^{-\sigma_1^2/\sigma_2^2}}{\pi\sigma_2^2\beta_1}\times\int_{v_0}^{\sigma_1/y_t}\frac{\mathrm{d}v}{v^3}\int_{\sin^{-1}(vy_t/\sigma_1)}^{\pi/2}S^2\exp\left[-\frac{\sigma_1^2 S^2}{\sigma_2^2 v^2}\right]\times\cosh\left[\frac{2\sigma_1^2 CS}{\sigma_2^2 v}\right]\mathrm{d}\theta_0. \quad (15)$$

Interchanging the order of integration we can rewrite (15) as

$$N_{t,v}^c(v_0)=\frac{4\sigma_1^2 e^{-\sigma_1^2/\sigma_2^2}}{\pi\sigma_2^2\beta_1}\int_{\sin^{-1}(v_0y_t/\sigma_1)}^{\pi/2}S^2\,\mathrm{d}\theta_0\times\int_{v_0}^{\sigma_1 S/y_t}\exp\left[-\frac{\sigma_1^2 S^2}{\sigma_2^2 v^2}\right]\times\cosh\left[\frac{2\sigma_1^2 CS}{\sigma_2^2 v}\right]\frac{\mathrm{d}v}{v^3}. \quad (16)$$

Making use of the transformation

$$\theta_0=\frac{\pi}{2}\varphi,\quad v=\frac{1}{x}, \quad (17)$$

we can rewrite (16) as

$$N_{t,v}^c(v_0)=\frac{2\sigma_1^2 e^{-\sigma_1^2/\sigma_2^2}}{\sigma_2^2\beta_1}\int_{(2/\pi)\sin^{-1}(v_0y_t/\sigma_1)}^{1}S_1^2\,\mathrm{d}\varphi\times\int_{y_t/\sigma_1 S_1}^{1/v_0}\exp\left[-\frac{\sigma_1^2}{\sigma_2^2}S_1^2x^2\right]\times\cosh\left[\frac{2\sigma_1^2 x\,C_1 S_1}{\sigma_2^2}\right]x\,\mathrm{d}x, \quad (18)$$

where S_1 and C_1 are defined to be

$$S_1=\sin\left(\frac{\pi}{2}\varphi\right),\quad C_1=\cos\left(\frac{\pi}{2}\varphi\right). \quad (19)$$

Carrying out the integration over x in (18) using the formula

$$\int_{r_1}^{r_2} x\, e^{-ax^2} \cosh(bx)\, dx = \frac{1}{4a}\left\{2\, e^{-ar_1^2}\cosh(br_1) - 2\, e^{-ar_2^2}\cosh(br_2) + \frac{\sqrt{\pi}}{2}\frac{b}{\sqrt{a}}\exp\left(\frac{b^2}{4a}\right) \times \left[\operatorname{erf}\left(\sqrt{a}r_2 - \frac{b}{2\sqrt{a}}\right) - \operatorname{erf}\left(\sqrt{a}r_2 + \frac{b}{2\sqrt{a}}\right) + \operatorname{erf}\left(\sqrt{a}r_1 + \frac{b}{2\sqrt{a}}\right) - \operatorname{erf}\left(\sqrt{a}r_1 - \frac{b}{2\sqrt{a}}\right)\right]\right\},$$

we obtain

$$N_{t,v}^c(v_0) = \frac{1}{2\beta_1}\int_{(2/\pi)\sin^{-1}(v_0 y_t/\sigma_1)}^{1} \left(2\, e^{-\sigma_1^2/\sigma_2^2} \times \left[e^{-y_t^2/\sigma_2^2}\cosh\left(\frac{2y_t\sigma_1 C_1}{\sigma_2^2}\right) - \exp\left(-\frac{\sigma_1^2 S_1^2}{\sigma_2^2 v_0^2}\right)\cosh\left(\frac{2\sigma_1^2 C_1 S_1}{\sigma_2^2 v_0}\right)\right] + \frac{\sqrt{\pi}\sigma_1}{\sigma_2} C_1 \exp\left(-\frac{\sigma_1^2 S_1^2}{\sigma_2^2}\right) \times\left\{\operatorname{erf}\left(\frac{y_t+\sigma_1 C_1}{\sigma_2}\right) - \operatorname{erf}\left(\frac{y_t-\sigma_1 C_1}{\sigma_2}\right) + \operatorname{erf}\left[\frac{\sigma_1}{\sigma_2}\left(\frac{S_1}{v_0} - C_1\right)\right] - \operatorname{erf}\left[\frac{\sigma_1}{\sigma_2}\left(\frac{S_1}{v_0} + C_1\right)\right]\right\}\right) d\varphi,$$

$$0 \le v_0 \le \sigma_1/y_t, \qquad (20)$$

which is to be evaluated numerically.

Many-atom ($P = MN$) *case*

The joint p.d.f. of v and y_N for this case has been shown to be [see (B1) of PP]

$$P(v,y_N) = \frac{4}{\sqrt{\pi}}\frac{y_N^2}{\sigma_1\sigma_2}\exp\left[-\frac{y_N^2(v^2+\sigma_1^2\sigma_2^2)}{\sigma_1^2\sigma_2^2}\right],$$

$$0 \le v < \infty, \quad 0 \le y_N < \infty. \qquad (21)$$

The joint p.d.f. of v and y_N applicable to the truncated data will therefore be given by [see (A4)]

$$P_t(v,y_N) = \frac{P(v,y_N)}{\beta_{MN}} = \frac{4}{\sqrt{\pi}\beta_{MN}}\frac{y_N^2}{\sigma_1\sigma_2}\exp[-\alpha^2 y_N^2],$$

$$0 \le v < \infty, \quad y_t \le y_N < \infty, \qquad (22)$$

where β_{MN} is the value of the c.c.f. of y_N for $y_N = y_t$ and α is defined by

$$\alpha^2 = \frac{v^2+\sigma_1^2\sigma_2^2}{\sigma_1^2\sigma_2^2}. \qquad (23)$$

Since y_N for the present case follows the acentric Wilson (1949) distribution, β_{MN} will be given by

$$\beta_{MN} = \int_{y_t}^{\infty} 2y_N \exp(-y_N^2)\, dy_N = \exp(-y_t^2). \qquad (24)$$

From (22) we obtain the p.d.f. of v valid for the truncated data to be

$$P_t(v) = \frac{4}{\sqrt{\pi}\beta_{MN}\sigma_1\sigma_2}\int_{y_t}^{\infty} y_N^2 \exp[-\alpha^2 y_N^2]\, dy_N. \qquad (25)$$

Changing the variable of integration from y_N to x by using the substitution $\alpha^2 y_N^2 = x$, then using the definition and the following properties of the incomplete gamma function (Abramowitz & Stegun, 1965)

$$\Gamma(a,x) + \gamma(a,x) = \Gamma(a)$$

$$\gamma\left(\frac{3}{2},x\right) = \frac{\sqrt{\pi}}{2}\operatorname{erf}(\sqrt{x}) - \sqrt{x}\exp(-x)$$

and finally substituting for α from (23) we obtain

$$P_t(v) = \frac{1}{\beta_{MN}}\left\{\frac{\sigma_1^2\sigma_2^2}{(v^2+\sigma_1^2\sigma_2^2)^{3/2}} + \frac{2y_t}{\sqrt{\pi}}\frac{\sigma_1\sigma_2}{(v^2+\sigma_1^2\sigma_2^2)} \times \exp\left[-\frac{(v^2+\sigma_1^2\sigma_2^2)y_t^2)}{\sigma_1^2\sigma_2^2}\right] - \frac{\sigma_1^2\sigma_2^2}{(v^2+\sigma_1^2\sigma_2^2)^{3/2}}\operatorname{erf}\left[\frac{(v^2+\sigma_1^2\sigma_2^2)^{1/2}}{\sigma_1\sigma_2}y_t\right]\right\}. \qquad (26)$$

The c.c.f. of v will therefore be given by

$$N_{t,v}^c(v_0) = 1 - N_{t,v}(v_0) = 1 - \int_0^{v_0} P_t(v)\, dv$$

$$= 1 - \frac{1}{\beta_{MN}}\left\{\int_0^{v_0}\frac{\sigma_1^2\sigma_2^2}{(v^2+\sigma_1^2\sigma_2^2)^{3/2}}dv + \int_0^{v_0}\left[\frac{2y_t}{\sqrt{\pi}}\frac{\sigma_1\sigma_2}{(v^2+\sigma_1^2\sigma_2^2)} \times \exp\left(-\frac{(v^2+\sigma_1^2\sigma_2^2)}{\sigma_1^2\sigma_2^2}y_t^2\right) - \frac{\sigma_1^2\sigma_2^2}{(v^2+\sigma_1^2\sigma_2^2)^{3/2}} \times \operatorname{erf}\left(\frac{(v^2+\sigma_1^2\sigma_2^2)^{1/2}}{\sigma_1\sigma_2}y_t\right)\right] dv\right\}. \qquad (27)$$

After evaluating the first integral on the r.h.s. of (27) we can rewrite (27) as

$$N_t^c(v_0) = 1 - \frac{1}{\beta_{MN}} \left(\frac{v_0}{(v_0^2 + \sigma_1^2 \sigma_2^2)^{1/2}} + \sigma_1 \sigma_2 \int_0^{v_0} \left\{ \frac{2y_t}{\sqrt{\pi}} \frac{1}{(v^2 + \sigma_1^2 \sigma_2^2)} \times \exp\left(-\frac{(v^2 + \sigma_1^2 \sigma_2^2)}{\sigma_1^2 \sigma_2^2} y_t^2 \right) - \frac{\sigma_1 \sigma_2}{(v^2 + \sigma_1^2 \sigma_2^2)^{3/2}} \times \operatorname{erf}\left[\frac{(v^2 + \sigma_1^2 \sigma_2^2)^{1/2}}{\sigma_1 \sigma_2} y_t \right] \right\} dv \right). \tag{28}$$

The above integral is to be evaluated numerically.

Many-atom ($P = MC$) *case*

The joint p.d.f. of v, y_N and θ_0 for this case is known to be [see (17) of PP]

$$P(v, y_N, \theta_0) = \frac{4\sqrt{2}}{\pi^{3/2} \sigma_1 \sigma_2^2} \frac{y_N^2}{S} \exp\left[-\frac{y_N^2}{\sigma_2^2} \left(1 + \frac{gv^2}{S^2} \right) \right] \times \cosh\left[\frac{2y_N^2 vC}{\sigma_2^2 S} \right], \tag{29}$$

where C and S are defined in (7) and g is defined by

$$g = \frac{1 + \sigma_1^2}{2\sigma_1^2}. \tag{30}$$

The joint p.d.f. of v, y_N and θ_0 applicable to the truncated data will therefore be given by [(see $A4$)]

$$P_t(v, y_N, \theta_0) = \frac{P(v, y_N, \theta_0)}{\beta_{MC}} = \frac{4\sqrt{2}}{\pi^{3/2} \sigma_1 \sigma_2^2 \beta_{MC}} \frac{y_N^2}{S} \times \exp\left[-\frac{y_N^2}{\sigma_2^2} \left(1 + \frac{gv^2}{S^2} \right) \right] \times \cosh\left[\frac{2y_N^2 vC}{\sigma_2^2 S} \right],$$

$$0 \le v < \infty, \quad y_t \le y_N < \infty, \; 0 \le \theta_0 \le \pi/2, \tag{31}$$

where β_{MC} is the value of the c.c.f. of y_N for $y_N = y_t$. From the p.d.f. of y_N for this case (see SP) we obtain

$$\beta_{MC} = 1 - \frac{2}{[\sigma_2^2(1 + \sigma_1^2)]^{1/2}} \int_0^{y_t} x \exp\left[-\frac{x^2}{\sigma_2^2(1 + \sigma_1^2)} \right] \times I_0\left[\frac{\sigma_1^2 x^2}{\sigma_2^2(1 + \sigma_1^2)} \right] dx. \tag{32}$$

The c.f. of v valid for the truncated data will therefore be given by

$$N_{t,v}(v_0) = \int_0^{v_0} \int_0^{\pi/2} \int_{y_t}^{\infty} P_t(v, y_N, \theta_0) \, dv \, dy_N \, d\theta_0. \tag{33}$$

Making use of (31) in (33) we obtain

$$N_{t,v}(v_0) = \frac{4\sqrt{2}}{\pi^{3/2} \sigma_1 \sigma_2^2 \beta_{MC}} \int_0^{\pi/2} \frac{d\theta_0}{S} \times \int_{y_t}^{\infty} y_N^2 \exp(-y_N^2/\sigma_2^2) \, dy_N \times \int_0^{v_0} \left\{ \exp\left[-\frac{gy_N^2 v^2}{\sigma_2^2 S^2} \right] \times \cosh\left[\frac{2y_N^2 Cv}{\sigma_2^2 S} \right] \right\} dv. \tag{34}$$

Carrying out the integration over v by the formula

$$\int_0^r e^{-ax^2} \cosh(bx) \, dx = \frac{\sqrt{\pi}}{4\sqrt{a}} \exp\left(\frac{b^2}{4a} \right) \times \left[\operatorname{erf}\left(\sqrt{a}r + \frac{b}{2\sqrt{a}} \right) + \operatorname{erf}\left(\sqrt{a}r - \frac{b}{2\sqrt{a}} \right) \right],$$

we obtain

$$N_{t,v}(v_0) = \frac{\sqrt{2}}{\pi \sigma_1 \sigma_2 \sqrt{g} \beta_{MC}} \int_0^{\pi/2} d\theta_0 \int_{y_t}^{\infty} y_N \times \exp\left[-\frac{y_N^2 (g - C^2)}{\sigma_2^2 g} \right] \times \left\{ \operatorname{erf}\left[\frac{y_N}{\sigma_2 \sqrt{g} S} (gv_0 + CS) \right] + \operatorname{erf}\left[\frac{y_N}{\sigma_2 \sqrt{g} S} (gv_0 - CS) \right] \right\} dy_N. \tag{35}$$

Making use of the substitution $y_N^2 = z$ and then using the transformations

$$z = \frac{x}{1 - x}, \quad \theta_0 = \frac{\pi\omega}{2}$$

and further employing the simplifying notation

$$\varphi(z,\theta_0) = \exp\left[-\frac{z(g-C^2)}{\sigma_2^2 g}\right] \times \left\{\operatorname{erf}\left[\left(\frac{z}{\sigma_2^2 g}\right)^{1/2}\left(\frac{gv_0+CS}{S}\right)\right] + \operatorname{erf}\left[\left(\frac{z}{\sigma_2^2 g}\right)^{1/2}\left(\frac{gv_0-CS}{S}\right)\right]\right\}, \quad (36)$$

we can rewrite (35) as

$$N_{t,v}(v_0) = \frac{1}{2\sqrt{2}\,\sigma_1\sigma_2\sqrt{g}\,\beta_{MC}} \times \int_0^1 \int_{y_t^2/(1+y_t^2)}^1 \varphi\left[\frac{x}{1-x}, \frac{\pi\omega}{2}\right]\frac{\mathrm{d}x\,\mathrm{d}\omega}{(1-x)^2}. \quad (37)$$

The c.c.f. of v will therefore be given by

$$N^c_{t,v}(v_0) = 1 - \frac{1}{2\sqrt{2}\,\sigma_1\sigma_2\sqrt{g}\,\beta_{MC}} \times \int_0^1 \int_{y_t^2/(1+y_t^2)}^1 \varphi\left[\frac{x}{1-x}, \frac{\pi\omega}{2}\right]\frac{\mathrm{d}x\,\mathrm{d}\omega}{(1-x)^2}. \quad (38)$$

The double integral on the r.h.s. of (38) is to be evaluated numerically.

4. Discussion of the theoretical results

By definition $N^c_{t,X}(X_0)$ denotes the fractional number of reflections for which $X \geq X_0$ relative to a population consisting of these reflections (in a given region of sin θ/λ) for which $y_N \geq y_t$. However, for discussing the effect of data truncation on the measurability of Bijvoet differences the more appropriate quantity is the fractional number of reflections for which $X \geq X_0$ and $y_N \geq y_t$ relative to the population consisting of *all* the theoretically possible independent reflections in the given range of sin θ/λ and we shall denote this fraction by the symbol $f_t(X_0)$. It is shown presently that $f_t(X_0)$ is functionally related to $N^c_{t,X}(X_0)$ so that $f_t(X_0)$ can be evaluated from a knowledge of $N^c_{t,X}(X_0)$.

Let n denote the number of all theoretically possible *independent* reflections within a given range of sin θ/λ in any particular crystal. Among these n reflections, let n_t be the number of reflections for which $y_N \geq y_t$. Among these n_t reflections let n_0 be the number of reflections for which $X \geq X_0$. Thus n_0 denotes the number of reflections for which $X \geq X_0$ and $y_N \geq y_t$ simultaneously. By definition we have

$$N^c_{t,X}(X_0) = n_0/n_t \quad (39)$$

and

$$N^c_{y_N}(y_t) = n_t/n, \quad (40)$$

where $N^c_{y_N}(y_t)$ denotes the value of the c.c.f. of y_N for $y_N = y_t$ corresponding to the untruncated data of the crystal. Since by definition $f_t(X_0) = (n_0/n)$ we can obtain from (39) and (40)

$$f_t(X_0) = (n_t/n)(n_0/n_t) = N^c_{y_N}(y_t)\,N^c_{t,X}(X_0). \quad (41)$$

It is obvious that $N^c_{y_N}(y_t)$ is the same as the quantity β_P ($P = 1$, MN and MC). Hence we can rewrite (41) as

$$f_t(X_0) = \beta_P N^c_{t,X}(X_0), \quad P = 1, MN \text{ and } MC. \quad (42)$$

For any given y_t, β_1 and β_{MC} can be evaluated numerically from (6) and (32) respectively and β_{MN} can be readily calculated from (24). For a given situation (*i.e.* $P = 1$, MN or MC) and given k, σ_1^2 and y_t, $N^c_{t,X}(X_0)$ would be equal to $N^c_{t,v}$ ($v = X_0/4k$) [see (3)]. The value of $N^c_{t,v}(X_0/4k)$ for given X_0, k, σ_1^2 and y_t can in turn be evaluated numerically from (20), (28) and (38) for the one-atom, many-atom ($P = MN$) and many-atom ($P = MC$) cases respectively. From the values of $N^c_{t,v}(X_0/4k)$ and β_P thus obtained the value of $f_t(X_0)$ for given X_0, σ_1^2, k and y_t can be evaluated [see (42)]. The values of $f_t(0{\cdot}05)$ thus obtained for the cases $P = 1$, MN and MC are given in Table 1 for different values of k and σ_1^2 corresponding to two typical values of y_t, namely $y_t = 0$* and 0·3. Table 2 contains the value of $f_t(0{\cdot}1)$ for the various cases.† To illustrate the general nature of the dependence of $f_t(0{\cdot}1)$ on y_t the curves of $f_t(0{\cdot}1)$ *vs* y_t for different fixed values of k and σ_1^2 are also shown in Fig. 1 for the many-atom (MN) case.

The quantity $f_t(0{\cdot}1)$ represents the fractional number of reflections for which the Bijvoet ratio $X \geq 0{\cdot}1$ and the normalized structure amplitude $y_N \geq y_t$ (which represents the truncation limit). For given P, σ_1^2 and k (*i.e.* for a given crystal and a given radiation) the curve of $f_t(0{\cdot}1)$ *vs* y_t has its maximum at $y_t = 0$ and the value of this maximum represents the quantity $N^c_X(0{\cdot}1)$ corresponding to the untruncated data. Thus each curve in Fig. 1 starts from the relevant value $N^c_X(0{\cdot}1)$ corresponding to the untruncated data and decreases systematically as y_t increases. This decrease is small initially (*e.g.* for $y_t \leq 0{\cdot}15$) and becomes rapid and practically linear for the middle range of values of y_t (*e.g.* $0{\cdot}3 \leq y_t < 1$). $f_t(0{\cdot}1)$ takes very low values for large values of y_t (*e.g.* $y_t > 1{\cdot}5$). This behaviour is to be expected physically.

It is interesting to see that in the one-atom case the behaviour of $f_t(0{\cdot}1)$ *vs* y_t differs somewhat for high and low values of σ_1^2. Thus, while for the situation $\sigma_1^2 < 0{\cdot}5$, the behaviour is similar to that obtained in the other cases, for the situation $\sigma_1^2 > 0{\cdot}7$ the value of $f_t(0{\cdot}1)$ is practically constant for low values of y_t. Thus, while the fractional number of reflections whose Bijvoet differences could be measured would decrease a little due to data truncation arising from unobserved

* This corresponds to the untruncated data.

† Tables of $f_t(0{\cdot}1)$ for y_t = 0, 0·15, 0·2, 0·3, ..., 1·5 are available in Ponnuswamy (1979).

reflections when $\sigma_1^2 < 0{\cdot}5$, this would remain practically unaffected when σ_1^2 is large.

The truncation limit y_t for actual data of crystals would generally be in the neighbourhood of 0·15 (Ponnuswamy & Parthasarathy, 1977). The Bijvoet difference data for the observed reflections whose intensities are close to this truncation limit may not be very accurate. Hence in our discussion we shall assume

Table 1. *The value of $f_t(0{\cdot}05)$ (in %) as a function of k and σ_1^2 for the cases P = 1, MN and MC when $y_t = 0$ and 0·3*

[$f_t(0{\cdot}05)$ denotes the fractional number of reflections for which $X \geq 0{\cdot}05$ and $y_N \geq y_t$.]

k ↓	P ↓	y_t ↓ σ_1^2 →	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
0.04	1	0.0	35.2	49.6	54.6	55.3	53.8	50.5	45.1	36.1	19.9
		0.3	27.7	42.0	47.1	48.3	47.6	45.6	41.8	34.8	19.8
	MN	0.0	27.9	38.4	43.7	46.2	47.0	46.2	43.7	38.4	27.9
		0.3	21.2	31.3	36.4	38.8	39.6	38.8	36.4	31.3	21.2
	MC	0.0	23.5	31.7	35.9	38.3	39.4	39.5	38.3	35.3	28.7
		0.3	21.5	28.9	32.7	34.7	35.6	35.3	33.9	30.6	23.9
0.06	1	0.0	54.9	65.7	68.3	68.3	67.0	64.3	59.9	52.4	37.0
		0.3	47.1	57.8	60.6	61.2	60.7	59.3	56.6	51.1	37.0
	MN	0.0	43.0	53.8	58.6	60.9	61.5	60.9	58.6	53.8	43.0
		0.3	35.7	46.2	50.9	53.1	53.7	53.1	50.9	46.2	35.7
	MC	0.0	35.8	44.8	49.4	52.0	53.3	53.6	52.7	50.0	42.9
		0.3	32.7	40.9	44.9	47.1	48.1	48.0	46.6	43.3	35.8
0.08	1	0.0	66.9	74.0	75.7	75.7	74.5	72.4	68.9	62.7	49.4
		0.3	58.9	66.0	67.9	68.4	68.1	67.3	65.5	61.4	49.3
	MN	0.0	53.8	63.6	67.7	69.6	70.2	69.6	67.7	63.6	53.8
		0.3	46.2	55.8	59.8	61.6	62.2	61.6	59.8	55.8	46.2
	MC	0.0	44.9	53.8	58.2	60.7	62.1	62.6	62.0	59.7	53.1
		0.3	41.0	49.1	52.9	55.0	56.0	56.0	54.8	51.8	44.3
0.10	1	0.0	73.9	79.1	80.4	80.3	79.4	77.6	74.7	69.5	58.1
		0.3	65.7	71.0	72.5	73.0	72.9	72.5	71.3	68.2	58.1
	MN	0.0	61.5	70.2	73.7	75.3	75.7	75.3	73.7	70.2	61.5
		0.3	53.7	62.2	65.6	67.2	67.6	67.2	65.6	62.2	53.7
	MC	0.0	51.7	60.2	64.3	66.7	68.1	68.6	68.3	66.4	60.7
		0.3	47.2	54.9	58.5	60.5	61.4	61.4	60.4	57.6	50.6
0.12	1	0.0	78.3	82.5	83.5	83.5	82.7	81.2	78.7	74.3	64.4
		0.3	70.1	74.4	75.7	76.1	76.2	76.0	75.3	72.9	64.3
	MN	0.0	67.2	74.8	77.8	79.2	79.6	79.2	77.8	74.8	67.2
		0.3	59.3	66.7	69.7	71.0	71.4	71.0	69.7	66.7	59.3
	MC	0.0	57.0	64.9	68.8	71.0	72.4	73.0	72.7	71.1	65.9
		0.3	52.0	59.2	62.6	64.4	65.3	65.3	64.3	61.7	54.9
0.14	1	0.0	81.5	85.0	85.8	85.8	85.1	83.8	81.6	77.8	69.2
		0.3	73.2	76.8	77.9	78.4	78.6	78.6	78.2	76.4	69.0
	MN	0.0	71.5	78.2	80.9	82.1	82.4	82.1	80.9	78.2	71.5
		0.3	63.4	70.0	72.6	73.8	74.2	73.8	72.6	70.0	63.4
	MC	0.0	61.1	68.6	72.2	74.3	75.6	76.2	76.0	74.6	69.6
		0.3	55.8	62.6	65.7	67.4	68.2	68.2	67.2	64.7	58.0
0.16	1	0.0	83.8	86.8	87.6	87.5	86.9	85.8	83.9	80.5	72.8
		0.3	75.5	78.6	79.7	80.1	80.4	80.6	80.5	79.1	72.7
	MN	0.0	74.8	80.8	83.2	84.3	84.6	84.3	83.2	80.8	74.8
		0.3	66.7	72.6	74.9	76.0	76.3	76.0	74.9	72.6	66.7
	MC	0.0	64.5	71.5	74.9	76.9	78.1	78.7	78.7	77.5	73.5
		0.3	58.9	65.2	68.2	69.7	70.5	70.5	69.6	67.2	61.3
0.18	1	0.0	85.6	88.3	89.0	88.9	88.3	87.3	85.6	82.6	75.7
		0.3	77.3	80.1	81.0	81.5	81.8	82.1	82.2	81.2	75.6
	MN	0.0	77.4	82.9	85.0	86.0	86.2	86.0	85.0	82.9	77.4
		0.3	69.3	74.6	76.7	77.6	77.9	77.6	76.7	74.6	69.3
	MC	0.0	67.2	73.9	77.1	79.0	80.2	80.8	80.9	80.1	77.2
		0.3	61.4	67.4	70.2	71.6	72.3	72.3	71.5	69.5	64.3
0.20	1	0.0	87.1	89.5	90.0	90.0	89.5	88.6	87.0	84.3	77.9
		0.3	78.7	81.2	82.1	82.6	83.0	83.4	83.6	82.9	78.0
	MN	0.0	79.6	84.6	86.5	87.3	87.6	87.3	86.5	84.6	79.6
		0.3	71.4	76.3	78.1	79.0	79.2	79.0	78.1	76.3	71.4
	MC	0.0	69.6	75.9	78.9	80.7	81.8	82.5	82.7	82.2	79.6
		0.3	63.6	69.2	71.8	73.2	73.8	73.8	73.1	71.2	66.4
0.22	1	0.0	88.2	90.4	90.9	90.9	90.4	89.6	88.2	85.2	79.7
		0.3	79.9	82.2	83.0	83.5	83.9	84.4	84.8	84.3	80.1
	MN	0.0	81.4	85.9	87.7	88.5	88.7	88.5	87.7	85.9	81.4
		0.3	73.1	77.6	79.3	80.1	80.3	80.1	79.3	77.6	73.1
	MC	0.0	71.6	77.6	80.4	82.2	83.3	83.9	84.1	83.6	81.1
		0.3	65.4	70.8	73.2	74.5	75.1	75.1	74.4	72.5	67.6
0.24	1	0.0	89.2	91.2	91.7	91.6	91.2	90.4	89.2	86.8	81.3
		0.3	80.8	82.9	83.7	84.2	84.7	85.2	85.8	85.5	81.9
	MN	0.0	82.9	87.1	88.7	89.4	89.6	89.4	88.7	87.1	82.9
		0.3	74.6	78.7	80.3	81.0	81.2	81.0	80.3	78.7	74.6
	MC	0.0	73.3	79.0	81.7	83.4	84.5	85.1	85.3	84.8	82.2
		0.3	67.0	72.1	74.4	75.6	76.2	76.1	75.4	73.5	68.5
0.26	1	0.0	90.0	91.9	92.3	92.3	91.9	91.2	90.0	87.8	82.9
		0.3	81.6	83.6	84.3	84.8	85.4	86.0	86.6	86.5	83.3
	MN	0.0	84.2	88.1	89.6	90.2	90.4	90.2	89.6	88.1	84.2
		0.3	75.9	79.7	81.2	81.8	82.0	81.8	81.2	79.7	75.9
	MC	0.0	74.8	80.3	82.9	84.4	85.5	86.0	86.2	85.6	83.0
		0.3	68.4	73.2	75.4	76.6	77.1	77.0	76.2	74.2	69.2
0.28	1	0.0	90.8	92.5	92.9	92.8	92.5	91.8	90.7	88.7	84.4
		0.3	82.3	84.2	84.9	85.4	85.9	86.6	87.3	87.4	84.4
	MN	0.0	85.3	88.9	90.3	90.9	91.1	90.9	90.3	88.9	85.3
		0.3	77.0	80.5	81.9	82.5	82.7	82.5	81.9	80.5	77.0
	MC	0.0	76.2	81.4	83.9	85.4	86.3	86.9	87.0	86.3	83.6
		0.3	69.6	74.2	76.3	77.4	77.9	77.7	76.9	74.8	69.7
0.30	1	0.0	91.4	93.0	93.3	93.3	93.0	92.3	91.3	89.5	85.8
		0.3	83.0	84.7	85.4	85.9	86.4	87.1	87.9	88.2	85.2
	MN	0.0	86.2	89.6	90.9	91.5	91.7	91.5	90.9	89.6	86.2
		0.3	77.9	81.2	82.5	83.1	83.2	83.1	82.5	81.2	77.9
	MC	0.0	77.4	82.4	84.7	86.2	87.1	87.5	87.6	86.9	84.1
		0.3	70.7	75.1	77.1	78.1	78.5	78.4	77.5	75.3	70.1

Table 2. *The value of $f_t(0{\cdot}10)$ (in %) as a function of k and σ_1^2 for the cases P = 1, MN and MC when $y_t = 0$ and 0·3*

[$f_t(0{\cdot}05)$ denotes the fractional number of reflections for which $X \geq 0{\cdot}10$ and $y_N \geq y_t$.]

k ↓	P ↓	y_t ↓ σ_1^2 →	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90
0.04	1	0.0	11.5	20.2	26.0	28.7	28.4	25.6	20.2	12.4	3.1
		0.3	4.7	8.5	10.6	11.7	12.0	11.5	10.2	8.0	4.2
	MN	0.0	9.8	15.7	19.3	21.3	21.9	21.3	19.3	15.7	9.8
		0.3	5.0	10.0	13.3	15.1	15.6	15.1	13.3	10.0	5.0
	MC	0.0	8.6	13.1	15.6	17.0	17.5	17.3	16.3	14.4	11.0
		0.3	5.2	13.4	19.2	22.2	22.7	21.0	17.3	11.3	3.0
0.06	1	0.0	23.0	36.3	42.7	44.5	43.3	39.8	34.0	24.8	10.4
		0.3	11.2	17.4	20.7	22.4	23.0	22.5	20.8	17.4	11.1
	MN	0.0	18.8	27.8	32.7	35.2	35.9	35.2	32.7	27.8	18.8
		0.3	12.8	21.2	25.8	28.2	29.0	28.2	25.8	21.2	12.8
	MC	0.0	16.2	22.9	26.6	28.6	29.5	29.4	28.1	25.4	20.0
		0.3	15.9	29.0	35.5	37.7	37.3	35.0	30.8	23.6	10.4
0.08	1	0.0	35.1	49.6	54.6	55.3	53.8	50.5	45.0	36.1	19.8
		0.3	17.9	25.5	29.4	31.5	32.3	31.9	30.1	26.3	18.4
	MN	0.0	27.8	38.4	43.6	46.2	47.0	46.2	43.6	38.4	27.8
		0.3	21.2	31.3	36.4	38.8	39.6	38.8	36.4	31.3	21.2
	MC	0.0	23.5	31.6	35.9	38.3	39.4	39.4	38.2	35.3	28.7
		0.3	27.7	42.0	47.1	48.3	47.6	45.6	41.8	34.8	19.8
0.10	1	0.0	46.0	59.1	62.6	62.8	61.4	58.4	53.4	45.2	29.0
		0.3	24.1	32.4	36.5	38.7	39.6	39.4	37.7	33.8	25.1
	MN	0.0	35.9	47.0	52.1	54.5	55.2	54.5	52.1	47.0	35.9
		0.3	29.0	39.6	44.5	46.9	47.6	46.9	44.5	39.6	29.0
	MC	0.0	30.1	38.9	43.4	45.9	47.2	47.3	46.3	43.4	36.3
		0.3	38.4	51.3	55.0	55.8	55.1	53.4	50.2	43.9	28.9
0.12	1	0.0	54.9	65.7	68.2	68.3	66.9	64.3	59.9	52.4	37.0
		0.3	29.4	38.0	42.2	44.5	45.5	45.3	43.7	39.9	31.0
	MN	0.0	42.9	53.8	58.6	60.8	61.5	60.8	58.6	53.8	42.9
		0.3	35.7	46.2	50.9	53.1	53.7	53.1	50.9	46.2	35.7
	MC	0.0	35.8	44.8	49.3	51.9	53.3	53.6	52.7	50.0	42.9
		0.3	47.1	57.8	60.6	61.2	60.7	59.3	56.6	51.1	37.0
0.14	1	0.0	61.7	70.4	72.4	72.4	71.2	68.8	64.9	58.1	43.7
		0.3	34.1	42.7	46.9	49.1	50.1	50.0	48.5	44.9	36.0
	MN	0.0	48.8	59.2	63.6	65.7	66.3	65.7	63.6	59.2	48.8
		0.3	41.4	51.5	55.8	57.8	58.4	57.8	55.8	51.5	41.4
	MC	0.0	40.7	49.7	54.2	56.7	58.1	58.5	57.8	55.3	48.4
		0.3	53.8	62.5	64.7	65.2	64.9	63.8	61.6	56.8	43.7
0.16	1	0.0	66.9	74.0	75.7	75.6	74.5	72.4	68.8	62.7	49.4
		0.3	38.1	46.6	50.7	52.9	53.9	53.8	52.5	49.0	40.3
	MN	0.0	53.8	63.6	67.7	69.6	70.1	69.6	67.7	63.6	53.8
		0.3	46.2	55.8	59.8	61.6	62.2	61.6	59.8	55.8	46.2
	MC	0.0	44.9	53.8	58.1	60.7	62.1	62.5	62.0	59.7	53.1
		0.3	58.9	66.0	67.9	68.4	68.1	67.3	65.5	61.4	49.3
0.18	1	0.0	70.8	76.8	78.2	78.2	77.2	75.2	72.0	66.4	54.1
		0.3	41.6	49.9	53.9	56.0	57.0	57.0	55.7	52.4	44.0
	MN	0.0	57.9	67.2	70.9	72.7	73.2	72.7	70.9	67.2	57.9
		0.3	50.3	59.3	63.0	64.7	65.2	64.7	63.0	59.3	50.3
	MC	0.0	48.5	57.2	61.4	63.9	65.3	65.8	65.4	63.3	57.1
		0.3	62.7	68.8	70.5	70.9	70.8	70.1	68.7	65.1	54.1
0.20	1	0.0	73.8	79.1	80.3	80.2	79.3	77.6	74.6	69.5	58.1
		0.3	44.6	52.7	56.5	58.6	59.6	59.6	58.4	55.3	47.2
	MN	0.0	61.5	70.1	73.6	75.2	75.7	75.2	73.6	70.1	61.5
		0.3	53.7	62.2	65.6	67.2	67.6	67.2	65.6	62.2	53.7
	MC	0.0	51.7	60.1	64.2	66.6	68.0	68.6	68.2	66.4	60.6
		0.3	65.7	71.0	72.5	73.0	72.9	72.5	71.3	68.2	58.1
0.22	1	0.0	76.3	80.9	82.1	82.0	81.1	79.5	76.8	72.1	61.5
		0.3	47.3	55.2	58.9	60.9	61.8	61.8	60.7	57.7	49.9
	MN	0.0	64.5	72.6	75.9	77.4	77.8	77.4	75.9	72.6	64.5
		0.3	56.7	64.6	67.8	69.2	69.7	69.2	67.8	64.6	56.7
	MC	0.0	54.5	62.7	66.6	69.0	70.3	70.9	70.6	68.9	63.5
		0.3	68.1	72.8	74.2	74.7	74.7	74.4	73.5	70.7	61.4
0.24	1	0.0	78.3	82.5	83.5	83.4	82.6	81.1	78.6	74.2	64.4
		0.3	49.7	57.3	60.9	62.8	63.7	63.7	62.6	59.7	52.0
	MN	0.0	67.2	74.8	77.8	79.2	79.6	79.2	77.8	74.8	67.2
		0.3	59.3	66.7	69.7	71.0	71.4	71.0	69.7	66.7	59.3
	MC	0.0	56.9	64.9	68.7	71.0	72.3	72.9	72.7	71.1	65.8
		0.3	70.1	74.4	75.7	76.1	76.2	76.0	75.3	72.9	64.3
0.26	1	0.0	80.0	83.8	84.7	84.7	83.9	82.5	80.2	76.1	66.9
		0.3	51.8	59.2	62.6	64.5	65.4	65.4	64.3	61.4	53.7
	MN	0.0	69.4	76.6	79.4	80.7	81.1	80.7	79.4	76.6	69.4
		0.3	61.5	68.5	71.3	72.5	72.9	72.5	71.3	68.5	61.5
	MC	0.0	59.1	66.8	70.5	72.7	74.0	74.6	74.4	72.9	67.7
		0.3	71.8	75.7	76.9	77.3	77.5	77.4	76.9	74.8	66.9
0.28	1	0.0	81.4	84.9	85.8	85.7	85.0	83.7	81.6	77.8	69.1
		0.3	53.7	60.8	64.2	66.0	66.8	66.8	65.8	63.0	55.4
	MN	0.0	71.4	78.2	80.8	82.0	82.4	82.0	80.8	78.2	71.4
		0.3	63.4	70.0	72.6	73.8	74.2	73.8	72.6	70.0	63.4
	MC	0.0	61.1	68.5	72.1	74.3	75.5	76.1	76.0	74.5	69.5
		0.3	73.2	76.8	77.9	78.4	78.6	78.6	78.2	76.4	69.0
0.30	1	0.0	82.7	85.9	86.7	86.7	86.0	84.6	82.8	79.2	71.1
		0.3	55.4	62.3	65.5	67.3	68.1	68.1	67.1	64.4	57.2
	MN	0.0	73.2	79.6	82.1	83.2	83.5	83.2	82.1	79.6	73.2
		0.3	65.2	71.4	73.9	75.0	75.3	75.0	73.9	71.4	65.2
	MC	0.0	62.8	70.1	73.6	75.6	76.9	77.5	77.4	76.1	71.4
		0.3	74.4	77.8	78.9	79.3	79.6	79.7	79.4	77.9	71.0

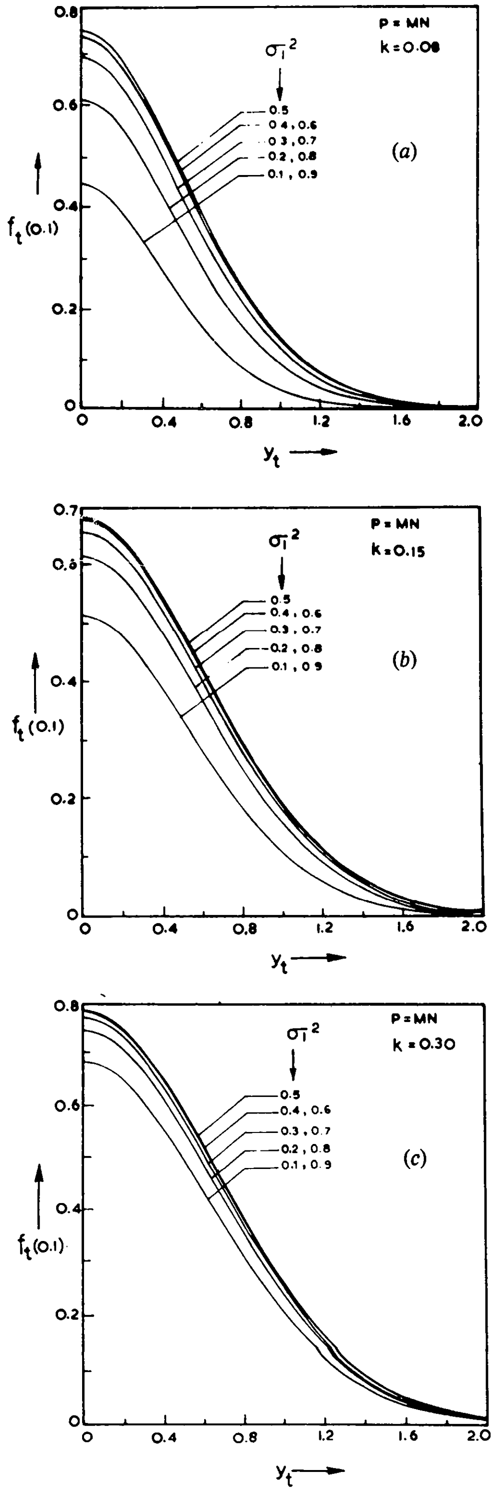

Fig. 1. The variation of $f_t(0\cdot1)$ as a function of the truncation limit y_t for different fixed values of σ_1^2 and k for the many-atom ($P = MN$) case. The curves (*a*), (*b*) and (*c*) are for $k = 0\cdot08$, $0\cdot15$ and $0\cdot3$ respectively. The numbers near the curves denote the value of σ_1^2. Note that $f_t(0\cdot1)$ denotes the fractional number of reflections for which $X \geq 0\cdot1$ and $y_N \geq y_t$.

that the Bijvoet difference data corresponding to reflections for which $y_N \geq 0\cdot3$ are sufficiently accurate to yield useful results. A study of Table 1 with this in view shows that a sufficient fractional number of observable reflections (*i.e.* $y_N > 0\cdot3$) would have Bijvoet ratios greater than 0·05 unless k is too small. For a typical situation in which k is low, $k \simeq 0\cdot08$, say (this is close to the mean value of k for Cl and Br for Cu $K\alpha$), and $P = 1$ and $\sigma_1^2 = 0\cdot2$, about 66% of the reflections are expected to have $X \geq 0\cdot05$ and $y_N \geq 0\cdot3$. For the same situation about 42% of the reflections are expected to have $X \geq 0\cdot1$ and $y_N > 0\cdot3$ (Table 2). For the situation where k is large, $k = 0\cdot22$, say (this is close to the mean value of k for I for Cu $K\alpha$ and Br for Mo $K\alpha$), and $P = 1$ and $\sigma_1^2 = 0\cdot2$, these numbers are 81 and 71% respectively. The results in Tables 1 and 2 thus indicate that though data truncation due to unobserved reflections would in general cause a decrease in the fractional number of reflections whose Bijvoet differences could be measured, it would not adversely affect the measurability of Bijvoet differences in a given crystal. That is, in spite of the unavoidable data truncation arising due to unobserved reflections, Bijvoet differences can be measured for a sufficiently large number of reflections for the purpose of phase determination by the anomalous scattering methods. This in turn implies that non-centrosymmetric structures containing hundreds of light atoms besides a few suitably chosen heavy atoms can be determined by exploiting the anomalous scattering phenomenon in an optimum way (Ramachandran & Parthasarathy, 1965) in spite of data truncation due to unobserved reflections.

It would be interesting to apply the results of our present theory for studying the measurability of Bijvoet

Table 3. *The value of* $f_t(X_0)$ (*in* %) *corresponding to* $X_0 = 0\cdot03$, $0\cdot05$ *and* $0\cdot1$ *as functions of* y_t *and* σ_1^2 *for the many-atom* ($P = MN$) *case when* $k = 0\cdot011$

y_t	x_0 ↓	σ_1^2: 0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.00	0.03	8.5	13.7	17.0	18.8	19.4
	0.05	3.3	5.7	7.3	8.2	8.5
	0.10	0.9	1.5	2.0	2.2	2.3
0.05	0.03	8.2	13.5	16.8	18.6	19.1
	0.05	3.1	5.5	7.0	7.9	8.2
	0.10	0.7	1.3	1.8	2.0	2.1
0.10	0.03	7.6	12.9	16.1	17.9	18.5
	0.05	2.6	4.9	6.4	7.3	7.6
	0.10	0.4	0.9	1.3	1.6	1.7
0.15	0.03	6.8	11.9	15.1	16.9	17.5
	0.05	2.0	4.1	5.6	6.5	6.8
	0.10	0.2	0.5	0.9	1.1	1.2
0.20	0.03	5.8	10.8	13.9	15.7	16.2
	0.05	1.4	3.3	4.7	5.6	5.8
	0.10	0.0	0.3	0.5	0.7	0.7
0.25	0.03	4.8	9.6	12.6	14.3	14.8
	0.05	0.9	2.5	3.8	4.6	4.8
	0.10	0.0	0.1	0.3	0.4	0.4
0.30	0.03	4.2	8.3	11.1	12.8	13.3
	0.05	0.5	1.9	3.0	3.6	3.9
	0.10	0.0	0.0	0.1	0.2	0.2

differences in light-atom structures. The values of $f_t(X_0)$ corresponding to $X_0 = 0{\cdot}03$, $0{\cdot}05$ and $0{\cdot}1$ and $y_t = 0, 0{\cdot}05, \ldots, 0{\cdot}3$ are given in Table 3 for the cases $P = MN$ by taking the value of k to be $0{\cdot}011$ which corresponds to the mean value for k for the O atom in the range $0 \le \sin\theta/\lambda \le 0{\cdot}5$ for Cu $K\alpha$ radiation. Results in Table 3 can be applied to light-atom structures containing only C and O since these have been computed on the assumption that k for C corresponding to Cu $K\alpha$ is very small compared to that for O. A study of this table shows that more than a dozen reflections can be found for which $X \ge 0{\cdot}05$ and $y_N \ge 0{\cdot}2$. This again shows that in spite of the data truncation due to unobserved reflections, Bijvoet differences could be measured for enough reflections for establishing the absolute configuration of an NC structure containing only light atoms by the Bijvoet method.

APPENDIX

Method of deriving probability density functions for truncated distributions

We can define different types of truncated distributions in multi-dimensional spaces since the concept of truncation can be applied to the interval of definition of each one of the random variables involved. However, in the text we meet with situations where truncation occurs for the interval associated with only one of the random variables defining the joint p.d.f. We shall therefore obtain presently the formula needed for deriving the truncated distribution for such a situation.

Let y_1 be a random variable with the p.d.f. $P(y_1)$ defined in $0 \le y_1 \le \infty$. Let $y_2, \ldots, y_N$ be random variables such that $P(y_1, y_2, \ldots, y_n)$, $0 \le y_i < \infty$ ($i = 1, 2, \ldots, n$), is the joint p.d.f. of $y_1, y_2, \ldots, y_{n-1}$ and y_n. Let $P_t(y_1, y_2, \ldots, y_n)$ be the joint p.d.f. for the truncated distribution when the random variable y_1 is restricted to lie in the interval* $y_1^t \le y_1 < \infty$. (Note that $0 \le y_i < \infty$ for $i = 2, 3, \ldots, n$.) That is,

$$\begin{aligned} P_t(y_1, y_2, \ldots, y_n) &\ne 0, \quad y_1^t \le y_1 < \infty, \\ &\qquad 0 \le y_i < \infty\,(i = 2, 3, \ldots, n) \\ &= 0 \text{ otherwise.} \end{aligned} \tag{A1}$$

The normalization condition for the truncated distribution defined in $y_1^t \le y_1 < \infty$, $0 \le y_i < \infty$, $i = 2, 3, \ldots,$ requires that $P_t(y_1, y_2, \ldots, y_n)$ be related to $P(y_1, y_2, \ldots, y_n)$ by

$$P_t(y_1, y_2, \ldots, y_n) = P(y_1, y_2, \ldots, y_n) \times \left[\int_{y_t}^{\infty}\int_0^{\infty}\int_0^{\infty} P(y_1, y_2, \ldots, y_n)\,dy_1, dy_2, \ldots, dy_n\right]^{-1}. \tag{A2}$$

We can rewrite the denominator of the expression on the r.h.s. of $(A2)$ as

$$\begin{aligned} &\int_{y_1^t}^{\infty}\int_0^{\infty}\ldots\int_0^{\infty} P(y_1, y_2, \ldots, y_n)\,dy_1, dy_2, \ldots, dy_n \\ &= \int_{y_1^t}^{\infty} dy_1 \int_0^{\infty}\ldots\int_0^{\infty} P(y_1, y_2, \ldots, y_n)\,dy_2, \ldots, dy_n \\ &= \int_{y_1^t}^{\infty} P(y_1)\,dy_1, \end{aligned} \tag{A3}$$

which follows since carrying out the $(n-1)$ integrations over the variables $y_2, y_3, \ldots, y_n$ leads finally to the marginal p.d.f. of y_1 (in $0 \le y_1 < \infty$). Making use of $(A3)$ in $(A2)$ we obtain

$$\begin{aligned} P_t(y_1, y_2, \ldots, y_n) &= \frac{P(y_1 y_2, \ldots, y_n)}{\int_{y_1^t}^{\infty} P(y_1)\,dy_2} \\ &= \frac{P(y_1, y_2, \ldots, y_n)}{\beta}, \end{aligned} \tag{A4}$$

say, where β is defined to be

$$\beta = \int_{y_1^t}^{\infty} P(y_1)\,dy_1. \tag{A5}$$

Making use of the normalization condition for the p.d.f. of y_1 we can also rewrite $(A5)$ as

$$\beta = 1 - \int_0^{y_1^t} P(y_1)\,dy_1 = 1 - N(y_1^t) = N^c(y_1^t), \tag{A6}$$

where $N(y_1^t)$ and $N^c(y_1^t)$ are respectively the values of the c.f. and c.c.f. of y_1 for $y_1 = y_1^t$.

It may be noted here that, for the sake of simplicity, we have taken the intervals from 0 to ∞. However it may be readily seen that $(A4)$ is valid even if the original intervals themselves are other than 0 to ∞ for some or all of the variables $y_2, \ldots, y_n$.

* Although we could define different types of truncated distributions based on the kind of truncation of the interval $0 \le y_1 < \infty$ we shall consider only one type of truncation, namely, the truncation of this interval at the lower end since we meet with such a kind of truncation only in this paper. For example, y_1 corresponds to the threshold value of the normalized structure amplitude y_N.

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Estimation of Experiment Time in Neutron Diffractometry of Large Structures. I. Anomalous Scattering

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Dedicated to Professor H. Jagodzinski on the occasion of his 65th birthday

Abstract

An *a priori* approach to the prediction of required neutron beam time for single-crystal analysis of biological structures is presented. Time economy is determined by several main features: (i) tolerable inaccuracy of the Fourier map, (ii) method of extracting phase information, (iii) data-collection technique. Phasing by anomalous scattering at two wavelengths is considered. An expression is derived for the error in scattering density arising from experimental intensity errors. Application of the theoretical probability distributions for the intensities leads to an equation for the expected total counting time. Conditions are established for which the time expenditure is a minimum. Tables which aid easy application of the results are given as well as a numerical example.

1. Introduction

The work of Schoenborn and his colleagues (Schoenborn, 1969; Norvell, Nunes & Schoenborn, 1975) has shown that neutron diffraction can be applied successfully to protein crystals. Protein neutron diffraction aims at the elucidation of structural features, particularly hydrogen atoms, which are not accessible to X-rays. The most serious problem of such work is the time and expense involved in data collection. In general, the practicability of a neutron study depends on the request for beam time.

Neutron diffraction offers the possibility of tackling the phase problem by means of anomalous scattering from nuclei such as ^{113}Cd, ^{149}Sm or ^{157}Gd. This method has been used to solve several small crystal structures (*e.g.* Koetzle & Hamilton, 1975; Sikka & Rajagopal, 1975). Results of an application to a protein structure have been reported by Schoenborn (1975).

The present paper is concerned with the prediction of experiment time when neutron anomalous scattering is used for phase determination. Its purpose is to provide a basis for experiment planning. The problem is approached by an analysis of the expected errors in the density map.

2. Tolerable density error

2.1. *Error model*

If series termination effects are not considered the true scattering density is defined by the truncated Fourier series

$$\rho(\mathbf{r}) = \bar{\rho} + V^{-1} \sum F_{\mathbf{H}} \cos (2\pi \mathbf{H}.\mathbf{r} - \varphi_{\mathbf{H}}), \qquad (1)$$

where V = unit-cell volume, $\bar{\rho} = F_0/V$ = average scattering density, $\varphi_{\mathbf{H}}$ = phase angle of structure factor $\mathbf{F}_{\mathbf{H}}$, $\mathbf{H}$ = reciprocal-lattice vector, and the summation is carried over a sphere in reciprocal space, up to a radius H_0.

The expected accuracy of the density can be predicted if a model for the errors in the Fourier components and a specific error criterion is assumed.

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