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The Effect of Coordinate Errors on the Phase-angle Distribution*

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The probability distribution of the magnitude of the phase-angle error ($|\theta^c|$) is worked out for an incomplete model structure when there are coordinate errors in the atomic positions. The corresponding problem for a centrosymmetric structure, namely the calculation of the percentage of reflexions for which the signs of the structure factors calculated from the coordinates of the model structure would agree with the true signs of the reflexions, is also worked out. The theoretical distributions could be used to study the effect of crystal-structure refinement on the phase-angle distribution. Numerical tables that are necessary for such a study are given.

Introduction

In an earlier paper (Parthasarathy, 1965*b*, hereafter referred to as P, 1965*b*) the probability distribution of θ ,[†] which is the difference in the phase of the true structure factor F_N arising from all the N atoms in the unit cell and that due to the atoms from an incomplete model structure containing $P (< N)$ atoms, has been worked out under the assumption that there are no errors in the coordinates of the atoms of the model. However, the model structure that is met with at any stage in a crystal-structure analysis is such that there are random errors in the coordinates of the atoms of the model and the process of crystal structure refinement consists in reducing this error as much as possible, consistent with the amount and accuracy of the intensity data. In this connexion it would be interesting to study how the probability distribution of the phase-angle difference is modified as the errors in the coordinates of the atoms in the model are reduced. In this paper we shall work out the probability distribution of the phase-angle error θ^c which is the difference

between the true phase of a reflexion and that (*i.e.* α_p^*) calculated from the coordinates of the atoms in the model structure. In order to avoid complications we shall consider only crystals and models which satisfy the requirements of the acentric distribution of Wilson (1949), namely the $P = MA$ case of P (1965*b*).

The corresponding problem for a centrosymmetric crystal would be (see Parthasarathy, 1965*a*, hereafter referred to as P, 1965*a*) the derivation of the probability function of s^c which is the product of the true sign s_N of the reflexion and that (*i.e.* s_p^*) calculated from the model structure. In this paper we shall also derive the probability function of s^c for crystals and models which satisfy the requirements of the centric distribution of Wilson (1949), namely the $P = M$ case of P (1965*a*).

Derivation of the probability distribution of θ^c

Consider a non-centrosymmetric crystal containing N atoms in the unit cell. Suppose that, at a given stage in a crystal-structure analysis, the model structure consists of $P (< N)$ atoms and let $\Delta \mathbf{r}_{Pj}$ be the error in the coordinates of atom j in the incomplete model. Following Luzzati (1952) we shall assume that the coordinate errors $\Delta \mathbf{r}_{Pj}$ ($j = 1, 2, \dots, P$) are normally distributed independent random vectors and define the quantity D to be

$$D = \langle \cos 2\pi \mathbf{H} \cdot \Delta \mathbf{r} \rangle_P \quad (1)$$

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† θ is also the phase-angle error since it is the amount by which the phase α_p of the model structure (without coordinate errors) is to be increased in order to obtain the true phase α_N of the reflexion.

where the average is over the coordinate errors of the atoms in the model structure.

From P (1965*b*) it is clear that the probability density function (abbreviated as p.d.f.) of θ^c can be obtained from a knowledge of the function $P(y_N, \theta^c; y_P^c)$ which is the conditional joint p.d.f. of y_N and θ^c for a given y_P^c (for notation employed see Srinivasan & Ramachandran, 1965). The function $P(y_N, \theta^c; y_P^c)$ can be easily obtained from the expression for the conditional joint p.d.f. of $|F_N|$ and θ^c for a given $|F_P^c|$ and the latter has been shown to be [see equation (A7), p. 8 of Srinivasan & Chandrasekaran (1966)]:

$$P(|F_N|, \theta^c; |F_P^c|) = \frac{1}{\pi} \frac{|F_N|}{[\sigma_Q^2 + \sigma_P^2(1-D^2)]} \times \exp \left[-\frac{(|F_N|^2 + D^2|F_P^c|^2 - 2|F_N||F_P^c|D \cos \theta^c)}{\sigma_Q^2 + \sigma_P^2(1-D^2)} \right]. \quad (2)$$

Making use of the normalized variables $y_N (= |F_N|/\sigma_N)$ and $y_P^c (= |F_P^c|/\sigma_P)$ and the notation that

$$\sigma_1^2 = \sigma_P^2/\sigma_N^2, \quad \sigma_2^2 = \sigma_Q^2/\sigma_N^2 \quad (3)$$

$$\sigma_A^2 = \sigma_1^2 D^2 \text{ and } \sigma_B^2 = \sigma_2^2 + \sigma_1^2(1-D^2), \quad (4)$$

we can rewrite equation (2) as

$$P(y_N, \theta^c; y_P^c) = \frac{y_N}{\pi \sigma_B^2} \times \exp \left[-\frac{(y_N^2 + \sigma_A^2 y_P^c{}^2 - 2\sigma_A y_N y_P^c \cos \theta^c)/\sigma_B^2}{\sigma_B^2} \right]. \quad (5)$$

In terms of the normalized variables y_N and $y_P (= |F_P|/\sigma_P)$ we can rewrite equation (5) of P (1965*b*) as

$$P(y_N, \theta; y_P) = \frac{y_N}{\pi \sigma_2^2} \times \exp \left[-\frac{(y_N^2 + \sigma_1^2 y_P^2 - 2\sigma_1 y_N y_P \cos \theta)/\sigma_2^2}{\sigma_2^2} \right]. \quad (6)$$

It is obvious from (3) and (4) that

$$\sigma_1^2 + \sigma_2^2 = 1 \text{ and } \sigma_A^2 + \sigma_B^2 = 1. \quad (7)$$

We know the p.d.f.'s of y_P^c and y_P to be

$$P(y) = 2y \exp[-y^2], \quad y = y_P \text{ or } y_P^c. \quad (8)$$

From the similarity of the pairs of expressions for $P(y_N, \theta^c; y_P^c)$ and $P(y_N, \theta; y_P)$ [see equations (5) and (6)] and those for $P(y_P^c)$ and $P(y_P)$ [see equations (8) and (7)] it is obvious that the p.d.f. of θ^c can be obtained from that of θ by replacing the set $(\theta, \sigma_1$ and $\sigma_2)$ by the corresponding set $(\theta^c, \sigma_A$ and $\sigma_B)$. We therefore obtain from equation (28) of P (1965*b*) the p.d.f. of $|\theta^c|$ to be

$$P(|\theta^c|) = \frac{\sigma_B^2}{\pi} + \frac{\sigma_A^2 \sigma_B^2 \cos^2 \theta^c}{\pi(1-\sigma_A^2 \cos^2 \theta^c)} + \frac{\sigma_A \sigma_B^2 \cos \theta^c}{(1-\sigma_A^2 \cos^2 \theta^c)^{3/2}} \times \left[\frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left\{ \frac{\sigma_A \cos \theta^c}{\sqrt{(1-\sigma_A^2 \cos^2 \theta^c)}} \right\} \right]. \quad (9)$$

Adding the first two terms in the right-hand side of (9) and replacing $\tan^{-1}(x)$ by its equivalent

$\sin^{-1}[x/\sqrt{1+x^2}]$ we can rewrite (9) as

$$P(|\theta^c|) = \frac{\sigma_B^2}{\pi(1-\sigma_A^2 \cos^2 \theta^c)} \left[1 + \frac{\sigma_A \cos \theta^c}{\sqrt{1-\sigma_A^2 \cos^2 \theta^c}} \times \left\{ \frac{\pi}{2} + \sin^{-1}(\sigma_A \cos \theta^c) \right\} \right]. \quad (10)$$

Derivation of the probability function of s^c

The probability function of s^c can be obtained from the conditional joint density function of y_N and s^c for a given y_P^c by following the procedure outlined in P (1965*a*).

From equation (A18) on p. 9 of Srinivasan & Chandrasekharan (1966) we obtain the conditional p.d.f. of F_N for a given F_P^c as

$$P(F_N; F_P^c) = \frac{\exp \left[\frac{-(F_N - DF_P^c)^2}{2\{\sigma_Q^2 + \sigma_P^2(1-D^2)\}} \right]}{\sqrt{2\pi\{\sigma_Q^2 + \sigma_P^2(1-D^2)\}}}. \quad (11)$$

We can therefore obtain the conditional joint p.d.f. of $|F_N|$ and s^c for a given $|F_P^c|$ to be [see equations (3), (4) (8) and (9) of P (1965*a*)]

$$P(|F_N|, s^c; |F_P^c|) = \frac{\exp \left[\frac{-(s|F_N| - D|F_P^c|)^2}{2\{\sigma_Q^2 + \sigma_P^2(1-D^2)\}} \right]}{\sqrt{2\pi\{\sigma_Q^2 + \sigma_P^2(1-D^2)\}}}. \quad (12)$$

Making use of the normalized variables y_N and y_P^c and (3) and (4), we can rewrite (12) as

$$P(y_N, s^c; y_P^c) = \frac{1}{\sqrt{2\pi\sigma_B^2}} \exp \left[-\frac{(s^c y_N - \sigma_A y_P^c)^2 / 2\sigma_B^2}{\sigma_B^2} \right]. \quad (13)$$

In terms of the normalized variables y_N and y_P we can rewrite equation (9) of P (1965*a*) as

$$P(y_N, s; y_P) = \frac{1}{\sqrt{2\pi\sigma_2^2}} \exp \left[-\frac{(s y_N - \sigma_1 y_P)^2 / 2\sigma_2^2}{\sigma_2^2} \right]. \quad (14)$$

The p.d.f.'s of y_P^c and y_P are known to be

$$P(y) = \sqrt{\frac{2}{\pi}} \exp[-y^2/2] \text{ where } y = y_P \text{ or } y_P^c. \quad (15)$$

From the similarity of the pairs of expressions for $P(y_N, s^c; y_P^c)$ and $P(y_N, s; y_P)$ [see equations (13) and (14)] and those for $P(y_P^c)$ and $P(y_P)$ [see equations (15) and (7)] it is obvious that the probability function of s^c can be obtained from that of s by simply replacing the set $(s, \sigma_1$ and $\sigma_2)$ by the corresponding set $(s^c, \sigma_A$ and $\sigma_B)$. We therefore obtain from equation (28) of P (1965*a*) the probability function of s^c as

$$P(s^c) = \frac{1}{2} + \frac{s^c}{\pi} \tan^{-1}[\sigma_A/\sigma_B] = \frac{1}{2} + \frac{s^c}{\pi} \sin^{-1}[\sigma_A]. \quad (16)$$

Discussion of the theoretical results

Making use of equations (3) and (4) in equation (10) we can obtain the cumulative function of $|\theta^c|$ as

$$N(|\theta^c|) = \int_0^{|\theta^c|} P(|\theta^c|) d\theta^c = \frac{(1 - \sigma_1^2 D^2)}{\pi} \times \int_0^{|\theta^c|} \left[1 + \frac{\sigma_1 D \cos \theta^c}{\sqrt{1 - \sigma_1^2 D^2 \cos^2 \theta^c}} \right] \times \left\{ \frac{\pi}{2} + \sin^{-1}(\sigma_1 D \cos \theta^c) \right\} \frac{d\theta^c}{(1 - \sigma_1^2 D^2 \cos^2 \theta^c)}. \quad (17)$$

The probability that the sign of F_p^s is the same as the true sign (i.e. for $s^c = +1$) can be obtained from equation (16) as

$$P(+)=P(s^c = +1) = \frac{1}{2} + \frac{1}{\pi} \sin^{-1}(\sigma_1 D) \quad (18)$$

where we have made use of equations (3) and (4). It is clear from (17) and (18) that quantities $N(|\theta^c|)$ and $P(+)$ depend on two parameters, namely σ_1^2 which is the fractional contribution to the local mean intensity from the atoms in the model structure, and D which is characteristic of the mean value of the magnitudes of the coordinate errors (i.e. $\langle |\Delta r| \rangle_p$) [see equation (19)]. As the number of atoms in the model structure increases, the value of σ_1^2 also increases and finally when the model accounts for all the N atoms in the structure the value of σ_1^2 tends to unity. As the crystal structure is refined more and more, the value of $\langle |\Delta r| \rangle$ decreases and hence that of D tends to unity. It is also readily seen that if we put $D=1$, equations (9) and (16) reduce respectively to equation (28) of P (1965b) and equation (28) of P (1965a) as required.

Luzzati (1952) has shown that the parameter D is related to the mean error $\langle |\Delta r| \rangle_p$ by the relation

$$D = \exp \left[- \frac{\pi^3}{4} H^2 \langle |\Delta r| \rangle^2 \right] \quad (19)$$

where H stands for $2(\sin \theta/\lambda)$. It is hence clear that the quantities $N(|\theta^c|)$ and $P(+)$ depend on $\langle |\Delta r| \rangle$ as well as the length H of the reciprocal lattice vector \mathbf{H} . It is convenient to obtain an average distribution for the whole set of data and hence we define a weighted-average cumulative function $\bar{N}(|\theta^c|)$ where the weight for a given H is taken to be the fractional number of reciprocal-lattice points in a thin shell of radius H and thickness dH . That is

$$\bar{N}(|\theta^c|) = \int_0^{H_{\max}} N(|\theta^c|) d\mathbf{H} / \int_0^{H_{\max}} d\mathbf{H} \quad (20)$$

where $d\mathbf{H}$ is the volume of the shell of radius H and thickness dH in reciprocal space. That is,

$$d\mathbf{H} = 4\pi H^2 dH. \quad (21)$$

In view of equation (21) we can rewrite equation (20) as

$$\bar{N}(|\theta^c|) = \frac{3}{H_{\max}^3} \int_0^{H_{\max}} N(|\theta^c|) H^2 dH \quad (22)$$

where H_{\max} is the largest value of H corresponding to the data at hand. For example, if the complete data for Cu $K\alpha$ is available then $H_{\max} = (2/1.542) = 1.297$.

In a similar way we define the average value for $\bar{P}(+)$ to be

$$\bar{P}(+) = \frac{1}{2} + \frac{3}{\pi H_{\max}^3} \int_0^{H_{\max}} \sin^{-1} \left[\sigma_1 \exp \left\{ - \frac{\pi^3}{4} \times H^2 \langle |\Delta r| \rangle^2 \right\} \right] H^2 dH. \quad (23)$$

The integrals in equations (22) and (23) are to be evaluated by a numerical method. For the equal-atom case, the value of σ_1^2 will be practically independent of H and hence can be taken to be a constant as far as the integration with respect to H is concerned. The values of $\bar{P}(+)$ and $\bar{N}(|\theta^c|)$ (for various values of $|\theta^c|$) were evaluated as a function of σ_1^2 and $\langle |\Delta r| \rangle$ and are given in Tables 1 and 2 respectively. The values of $\bar{P}(+)$ and $\bar{N}(|\theta^c|)$ corresponding to $\langle |\Delta r| \rangle = 0$ agree with the values of $P(+)$ and $N(\theta)$ (see P, 1965a, b) respectively as is to be expected.

It may be noted here that equations (22) and (23) also hold good for crystals containing a sufficiently large number of heavy atoms at general positions in the model structure such that F_p^s follows a Wilson distribution. However, in this case σ_1^2 will be a slowly varying function of H and for a rigorous evaluation of the average functions $\bar{N}(|\theta^c|)$ and $\bar{P}(+)$ this fact must also be taken into account. Since this makes the numerical evaluation of equations (22) and (23) more difficult we shall not attempt it here. A more convenient method of handling such cases would be to compute the average value of σ_1^2 from the known contents of the unit cell and model structure [see P (1965a) for the procedure for obtaining the average value of σ_1^2] and make use of this value to obtain the distributions from Tables 1 and 2.

A study of Table 1 shows that when σ_1^2 is not very large, the value of $\bar{P}(+)$ remains practically the same when $\langle |\Delta r| \rangle$ varies in the range 0 to 0.1 Å. This shows that when the mean error in the model structure is

Table 1. Values of $\bar{P}(+)$ for different values of $\langle |\Delta r| \rangle$ and σ_1^2

$\langle \Delta r \rangle / \sigma_1^2$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.00	60.2	64.8	68.5	71.8	75.0	78.2	81.5	85.2	89.8	100.0
0.05	60.2	64.6	68.3	71.6	74.8	77.9	81.2	84.8	89.1	96.3
0.05	60.0	64.5	68.0	71.3	74.4	77.5	80.6	84.1	88.1	95.9
0.08	59.7	64.0	67.4	70.6	73.5	76.4	79.3	82.4	85.9	90.5
0.10	59.5	63.6	66.9	69.9	72.7	75.5	78.2	81.1	84.2	88.0
0.15	58.6	62.5	65.3	67.9	70.3	72.7	74.9	77.3	79.7	82.3
0.20	57.5	60.7	63.3	65.5	67.6	69.5	71.4	73.2	75.1	77.0
0.30	55.3	57.5	59.2	60.7	62.1	63.3	64.5	65.7	66.8	67.9
0.40	53.4	54.8	55.9	56.8	57.7	58.5	59.2	59.9	60.6	61.2
0.50	52.1	53.0	53.6	54.2	54.7	55.2	55.6	56.1	56.5	56.9
0.60	51.3	51.8	52.2	52.6	52.9	53.2	53.5	53.7	54.0	54.2
0.80	50.5	50.8	51.0	51.1	51.3	51.4	51.5	51.6	51.7	51.8
1.00	50.3	50.4	50.5	50.6	50.6	50.7	50.8	50.8	50.9	50.9

Table 2. Cumulative function $\bar{N}(|\theta^c|)$ for different values of $\langle|\Delta r|\rangle$ and σ_1^2
 θ^c is in degrees and $\langle|\Delta r|\rangle$ in Å.

$\langle \Delta r \rangle/\sigma^c$	3	6	10	15	20	30	40	60	90	120	150	180
SIGMA SQUARE = 0.2												
0.00	3.4	6.7	11.1	16.6	21.9	31.9	40.9	56.1	72.4	85.7	92.4	100
0.03	3.3	6.7	11.1	16.5	21.8	31.7	40.8	55.9	72.2	83.6	92.3	100
0.05	3.3	6.6	11.0	16.3	21.6	31.5	40.5	55.6	71.9	83.4	92.2	100
0.08	3.2	6.5	10.7	16.0	21.1	30.9	39.7	54.8	71.3	82.9	92.0	100
0.10	3.2	6.3	10.5	15.7	20.8	30.3	39.1	54.1	70.7	82.5	91.9	100
0.15	3.0	6.0	9.9	14.8	19.6	28.7	37.2	51.9	68.8	81.7	91.2	100
0.20	2.8	5.6	9.3	13.8	18.5	26.9	35.0	49.4	66.5	79.6	90.3	100
0.30	2.4	4.8	8.0	11.9	15.9	23.5	30.8	44.4	61.6	76.0	88.4	100
0.40	2.1	4.2	7.1	10.6	14.0	20.9	27.6	40.3	57.5	72.8	85.4	100
0.50	1.9	3.9	6.5	9.7	12.9	19.2	25.5	37.6	54.6	70.5	85.4	100
0.60	1.8	3.7	6.1	9.2	12.2	18.2	24.2	35.9	52.9	69.0	84.6	100
0.80	1.7	3.5	5.8	8.7	11.6	17.5	23.1	34.6	51.2	67.7	83.9	100
1.00	1.7	3.4	5.7	8.5	11.4	17.0	22.7	33.9	50.6	67.2	83.6	100
SIGMA SQUARE = 0.4												
0.00	4.7	9.4	15.6	23.0	30.0	42.5	52.9	68.2	81.6	89.6	95.3	100
0.03	4.7	9.3	15.4	22.8	29.8	42.2	52.6	67.8	81.4	89.5	95.2	100
0.05	4.6	9.2	15.2	22.5	29.3	41.7	52.0	67.2	80.8	89.2	95.1	100
0.08	4.4	8.9	14.7	21.7	28.4	40.5	50.7	66.0	80.1	88.7	94.8	100
0.10	4.3	8.6	14.2	21.0	27.6	39.4	49.5	64.9	79.2	88.1	94.5	100
0.15	3.9	7.8	12.9	19.2	25.2	36.3	46.0	61.4	76.6	86.5	93.7	100
0.20	3.5	7.0	11.6	17.3	23.0	33.0	42.2	57.4	73.3	84.5	91.7	100
0.30	2.8	5.6	9.4	14.0	18.5	27.2	35.3	49.5	66.4	79.5	90.2	100
0.40	2.4	4.7	7.9	11.7	15.6	23.1	30.2	43.4	60.6	75.1	87.9	100
0.50	2.1	4.2	6.9	10.0	13.8	20.5	27.0	39.5	56.5	71.9	86.2	100
0.60	1.9	3.8	6.4	9.6	12.8	19.0	25.2	37.1	54.0	69.9	85.1	100
0.80	1.8	3.6	5.9	8.9	11.8	17.7	23.5	35.0	51.7	68.1	83.1	100
1.00	1.7	3.4	5.7	8.6	11.5	17.2	22.9	34.2	50.4	67.4	83.7	100
SIGMA SQUARE = 0.6												
0.00	6.7	13.2	21.7	31.6	40.3	55.0	65.7	78.9	88.7	95.8	97.2	100
0.03	6.6	13.0	21.4	31.1	39.9	54.4	65.1	78.5	88.5	95.7	97.3	100
0.05	6.4	12.7	20.8	30.4	39.1	53.4	64.1	77.7	88.0	95.4	97.0	100
0.08	6.0	12.0	19.7	28.8	37.1	51.2	61.9	75.9	86.8	92.7	96.7	100
0.10	5.7	11.4	18.8	27.5	35.8	49.3	60.0	74.5	85.8	92.1	96.4	100
0.15	5.0	9.9	16.4	24.1	31.4	44.2	54.6	69.7	82.6	90.2	95.5	100
0.20	4.3	8.5	14.1	20.9	27.4	39.0	49.0	64.3	78.6	87.7	94.3	100
0.30	3.2	6.5	10.7	16.0	21.0	30.6	39.2	53.9	70.1	82.0	91.5	100
0.40	2.6	5.2	8.6	13.8	17.9	25.0	32.5	46.0	62.9	76.8	88.8	100
0.50	2.2	4.4	7.4	11.0	14.6	21.6	28.4	41.0	58.0	73.0	86.8	100
0.60	2.0	4.0	6.7	10.0	13.2	19.7	26.0	38.1	54.9	70.6	85.5	100
0.80	1.8	3.6	6.0	9.0	12.0	18.0	23.8	35.4	52.1	68.4	84.3	100
1.00	1.7	3.5	5.8	8.7	11.6	17.3	23.1	34.4	51.1	67.5	83.8	100
SIGMA SQUARE = 0.8												
0.00	10.5	20.7	33.2	46.6	57.3	72.0	80.7	89.5	94.7	97.2	98.7	100
0.03	10.2	20.1	32.3	45.4	56.0	70.8	79.7	88.9	94.4	97.0	98.7	100
0.05	9.7	19.1	30.7	43.8	54.9	69.9	78.2	87.8	93.9	96.7	98.5	100
0.08	8.7	17.2	27.8	39.7	49.8	64.9	74.6	85.4	91.4	95.3	97.9	100
0.10	8.0	15.8	25.8	37.0	46.7	61.7	71.8	83.4	91.4	95.3	97.9	100
0.15	6.5	12.8	21.0	30.5	39.2	53.3	63.8	77.3	87.6	93.2	96.9	100
0.20	5.3	10.5	17.2	25.3	32.7	45.6	55.9	70.5	83.0	90.4	95.6	100
0.30	3.7	7.4	12.2	18.0	23.7	36.0	43.1	57.7	73.2	84.1	92.5	100
0.40	2.8	5.7	9.4	14.0	18.4	26.9	34.7	48.4	64.9	78.7	89.5	100
0.50	2.3	4.7	7.8	11.6	15.4	22.7	29.6	42.4	59.2	73.9	87.3	100
0.60	2.1	4.2	6.9	10.3	13.7	20.3	26.8	38.0	55.7	71.7	85.8	100
0.80	1.8	3.7	6.1	9.2	12.2	18.2	24.2	35.7	52.5	68.6	84.4	100
1.00	1.8	3.5	5.9	8.8	11.7	17.5	23.2	34.6	51.3	67.7	83.9	100
SIGMA SQUARE = 1.0												
0.00	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100
0.01	80.5	95.6	97.5	98.8	99.3	99.7	99.8	99.9	99.9	99.9	99.9	100
0.02	57.6	80.5	91.2	95.7	97.4	98.8	99.3	99.7	99.8	99.9	99.9	100
0.03	43.3	67.8	83.1	91.1	94.6	97.4	98.4	99.2	99.6	99.8	99.9	100
0.04	34.3	57.4	75.0	85.7	90.9	95.5	97.3	98.7	99.4	99.7	99.9	100
0.05	28.2	49.3	67.5	80.1	88.9	93.2	95.8	98.0	99.0	99.5	99.8	100
0.06	23.9	43.0	60.9	74.6	82.6	90.6	94.2	97.1	98.6	99.3	99.7	100
0.07	20.7	37.9	55.2	69.4	78.3	87.8	92.3	96.1	98.1	99.0	99.6	100
0.08	18.2	33.8	50.2	64.6	74.2	84.9	90.3	95.0	97.6	98.7	99.4	100
0.09	16.2	30.5	46.0	60.2	70.1	81.9	88.1	93.7	96.9	98.4	99.3	100
0.10	14.6	27.7	42.3	56.2	66.3	79.0	85.8	92.4	96.3	98.0	99.1	100
0.15	9.6	18.6	29.5	41.2	50.8	60.9	74.2	84.8	92.1	95.7	98.1	100
0.20	7.0	13.7	22.1	31.6	39.9	55.4	63.4	76.5	86.9	92.7	96.7	100
0.30	4.4	8.7	14.2	20.8	26.9	37.8	47.0	61.4	76.0	85.8	93.4	100
0.40	3.2	6.3	10.4	15.3	20.0	28.8	36.8	50.6	66.7	79.4	90.2	100
0.50	2.5	5.0	8.3	12.4	16.3	23.8	30.9	43.7	60.3	74.7	87.7	100
0.60	2.2	4.4	7.2	10.8	14.3	21.0	27.5	39.7	56.4	71.7	86.0	100
0.80	1.9	3.8	6.3	9.4	12.5	18.5	24.5	36.1	52.8	68.9	84.5	100
1.00	1.8	3.6	5.9	8.9	11.8	17.6	23.4	34.7	51.4	67.8	83.9	100

about 0.1 Å, it is not very rewarding to refine the incomplete model structure first and then use the refined coordinates to calculate a Fourier synthesis to locate

more atoms [see Ramachandran & Srinivasan (1961) for the relative importance of phase over structure-factor magnitude in Fourier synthesis]. In other words, we can proceed with the process of structure completion first (*i.e.* locating more and more atoms from the subsequent Fourier maps), thereby making the value of σ_1^2 larger and larger, and finally refine the complete but imperfect model structure. It can be seen from Table 1 that when $\sigma_1^2=1$ and $\langle|\Delta r|\rangle=0.1$ Å, the value of $\bar{P}(+)$ is 88% and this shows that at this stage 12% of reflexions will still have their signs different from that of the model structure. Since, when $\sigma_1^2=1$, the value of $\bar{P}(+)$ increases noticeably with decrease in the value of $\langle|\Delta r|\rangle$ the refinement at this stage would be meaningful and rapid.

A study of Table 2 shows that even in non-centrosymmetric crystals similar conclusions hold good, namely (i) that it may not be advantageous to refine an incomplete structure (provided the errors in the coordinates are about 0.1 Å) and then proceed with structure completion, and (ii) the refinement of a completed (*i.e.* $\sigma_1^2=1$) but imperfect structure would be meaningful and rapid.

A study of the values of $\bar{N}(90^\circ)$ in Table 2 shows that provided the value of the mean error in the coordinates of the anomalous scatterer is not more than 0.1 Å the percentage of reflexions whose phases are correctly determined by the quasi-anomalous method (see P, 1965b) remains practically the same as when there are no errors in the coordinates of the anomalous scatterer.

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