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Estimation of the Mean Error in Atomic Positions from the Overall Values of *R* Indices

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Abstract

The theoretical overall values of different types of R indices have been evaluated as a function of the mean coordinate error (*i.e.* $\langle|\Delta\mathbf{r}|\rangle$) for the atoms in a model and the fractional contribution of the known atoms to the local mean intensity (*i.e.* σ_1^2). The effect of data truncation due to unobserved reflections has also been taken into account. Results for centrosymmetric and non-centrosymmetric crystals containing similar atoms have been obtained in the form of compact tables. Results in these tables can be used to obtain the mean coordinate error $\langle|\Delta\mathbf{r}|\rangle$ for any model from the overall values of the R indices.

1. Introduction

Ramachandran and co-workers derived the joint probability density function (p.d.f.) of the structure factor (F_N, say) of the 'true' structure containing N atoms and the calculated structure factor (F_P^c, say) of an 'assumed model' containing a part P of the atoms ($P \leq N$) with coordinate errors and used it to deduce a number of crystallographic results [for details see the monograph of Srinivasan & Parthasarathy (1976)]. They considered the following two situations: (i) situation I: a centrosymmetric model of a centrosymmetric structure and (ii) situation II: a non-centrosymmetric model of a non-centrosymmetric structure. Later, Swaminathan & Srinivasan (1975) worked out the joint p.d.f. of F_N and F_P^c of a centrosymmetric model of a non-centrosymmetric crystal which is approximately centrosymmetric.

Using the joint p.d.f. of F_N and F_P^c available in the literature, Parthasarathy and co-workers have tabulated the local values of six normalized R indices as a function of the parameter D [see (3) for a definition of D which is a function of both $(\sin\theta)/\lambda$ and the mean coordinate error† (*i.e.*, $\langle|\Delta\mathbf{r}|\rangle$) for the atoms in the assumed model] and have suggested a method for computing the theoretical overall values of the normalized R indices for any given value of $\langle|\Delta\mathbf{r}|\rangle$ (Parthasarathy & Velmurugan, 1981; Velmurugan & Parthasarathy, 1981*a*). They have also worked out the corresponding theoretical results for six types of unnormalized R indices (Velmurugan & Parthasarathy, 1981*b*). However, so far no convenient tables of overall values of R indices as a function of $\langle|\Delta\mathbf{r}|\rangle$ and σ_1^2 [which represents the fraction of the true structure accounted for by the assumed model, see (2) for the definition of σ_1^2] are available in the literature. Such a table would be very useful in practice since it enables one easily to obtain the mean coordinate error $\langle|\Delta\mathbf{r}|\rangle$ for an assumed model from the observed overall value of any of the R indices. In this paper we shall deal with this problem for situations I and II. The theoretical results for the third situation, namely, a centrosymmetric model of a non-centrosymmetric crystal which is approximately centrosymmetric will be dealt with separately.

It is possible to calculate R indices using directly either the normalized structure-factor magnitude variables or the normalized intensity variables instead of $|F_N|$ and $|F_P^c|$. This enables us to define six other types of normalized R indices (see Parthasarathy, 1987) and these have not been considered in the earlier papers. We shall therefore obtain the theoretical values of eighteen different types of R indices as a function of $\langle|\Delta\mathbf{r}|\rangle$ and σ_1^2 in the form of compact tables.

In this paper we shall follow the notation and nomenclature used by Parthasarathy (1987) with some minor modifications. We shall denote R indices calculated using truncated data (*i.e.* data for which the reflections which are too weak to be observed are omitted) with a subscript t to the variable used for calculating the R index. For example, $\bar{R}_1(F_t)$† is the overall value of the normalized conventional R index based on F computed using data from which the reflections with $|F_N| < F_t$ (= the threshold value for structure-factor magnitudes) are excluded.

2. Derivation of the theoretical expressions for the overall values of *R* indices

Consider a crystal (space group $P1$ or $P\bar{1}$) containing a large number (N, say) of similar atoms in the unit cell. During any stage of structure analysis, let the

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† $\langle|\Delta\mathbf{r}|\rangle = (1/P)\sum_{j=1}^{P}|\Delta\mathbf{r}|$. For convenience we shall hereafter refer to $\langle|\Delta\mathbf{r}|\rangle$ as the mean error in the atomic positions for the model.

† This was denoted earlier by the more cumbersome symbol $[\bar{R}_1(F)]_t$ (see Parthasarathy & Velmurugan, 1981).

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proposed model consist of P ($<N$) atoms. Let $\langle|\Delta\mathbf{r}|\rangle$ be the mean error in the positions of the atoms in the model. Let $|F_N|$ be the structure-factor magnitude of a reflection H ($=hkl$) for the true structure and let $|F_P^c|$ be the corresponding calculated value for the model. Let y_N and y_P^c be the normalized structure-amplitude variables associated with $|F_N|$ and $|F_P^c|$, respectively. That is,

$$y_N = |F_N|/\langle|F_N|^2\rangle^{1/2} = |F_N|/\sigma_N,$$
$$y_P^c = |F_P^c|/\langle|F_P^c|^2\rangle^{1/2} = |F_P^c|/\sigma_P^c, \quad (1)$$

where $\sigma_N^2 = \langle|F_N|^2\rangle$ and $(\sigma_P^c)^2 = \langle|F_P^c|^2\rangle$. Let σ_1^2 be the fractional contribution to the local mean intensity from the P atoms of the model.

$$\sigma_1^2 = \langle|F_P^c|^2\rangle/\langle|F_N|^2\rangle. \quad (2)$$

Following Luzzati (1952), we shall define D as

$$D = \langle\cos 2\pi\mathbf{H}\,.\,\Delta\mathbf{r}\rangle. \quad (3)$$

Assuming $\Delta\mathbf{r}$ to follow a three-dimensional Gaussian distribution, Luzzati (1952) showed that

$$D = \exp[-(\pi^3/4)H^2\langle|\Delta\mathbf{r}|\rangle^2]. \quad (4)$$

Following Srinivasan & Ramachandran (1966), we define σ_A and σ_B as

$$\sigma_A = \sigma_1 D, \qquad \sigma_B = (1-\sigma_A^2)^{1/2}. \quad (5)$$

Let F_t be the threshold value of $|F_N|$ and let y_t be the corresponding threshold value of y_N.

The notation and definition of various R indices are given in Table 1. The procedure employed by Parthasarathy & Velmurugan (1981) for obtaining the theoretical expressions for the overall values of R indices consists of the following steps: (i) Rewrite the defining equation for the overall value of R* in term of the normalized variables y_N and y_P^c. (ii) Partition the reciprocal space into sufficiently thin shells so that the atomic scattering factor corresponding to various reflections in any given shell may be treated as constant. (iii) Write the sum over all the observed reflections as a summation over those reflections which lie in a given shell and then sum over the contributions from the various shells. The final expressions for the various R indices as obtained in the earlier papers (Parthasarathy & Velmurugan, 1981; Velmurugan & Parthasarathy, 1981*a*, *b*) are summarized in the fourth column of Table 1. The procedure suggested in these papers for evaluating the theoretical overall values are inconvenient owing to the presence of the crystal-dependent quantity n_s (=the number of observed reflections in the sth shell). This difficulty may be overcome by a simple procedure consisting of dividing the reciprocal space into equi-volume shells instead of shells of arbitrary volumes. We shall consider this aspect presently.

* We use R and $\bar{R}$ to denote, respectively, a local value and the overall value of any one of the R indices.

Suppose that we partition the region $0 \le H \le H_{max}$ of the reciprocal space* into ν thin shells of equal volume. We may then take n_s to be practically the same in the various shells so that we can cancel out n_s from the numerator and denominator of the expression of any given R index. The final expressions thus obtained for the overall values of the R indices are given in the fifth column of Table 1.

3. Method of computing the theoretical overall values of R indices

It is seen from the theoretical expression for $\bar{R}$ given in Table 1 that the computation of the theoretical overall value of R for a given model would involve the following steps: (i) Partitioning the reciprocal space into ν equi-volume shells and finding the mean value of $(\sin\theta)/\lambda$ for each shell. Let $\bar{s}_i$ be the mean value of $(\sin\theta)/\lambda$ for the ith shell ($i = 1, 2, \ldots, \nu$). (ii) Obtaining the scattering factor for an average atom for the structure. (iii) Calculating the local values of the R index and the weights corresponding to the various shells (*i.e.* corresponding to the values $\bar{s}_1, \bar{s}_2, \ldots, \bar{s}_\nu$). (iv) Computing the overall value of the R index by making use of the values obtained in steps (i) to (iii) in the appropriate equation for the overall value of the R index given in Table 1. In §§ 3.1 to 3.3 we shall consider the computational aspects involved in steps (i)–(iii).

3.1. *An algorithm for partitioning the region $H_{min} \le H \le H_{max}$ of the reciprocal space into ν equi-volume shells*

The radii of the boundaries of the spherical shells and the mean values of $(\sin\theta)/\lambda$ corresponding to the various shells when the region of reciprocal space $H_{min} \le H \le H_{max}$ is partitioned into ν equi-volume shells can be obtained as follows.

Let V_0 be the total volume of the region $H_{min} \le H \le H_{max}$ of the reciprocal space so that

$$V_0 = \tfrac{4}{3}\pi(H_{max}^3 - H_{min}^3). \quad (6)$$

If this region is partitioned into ν shells of equal volume, then the volume of each shell is V_0/ν. If H_i and H_{i+1} are respectively the inner and outer radii of the ith shell, then the volume of the ith shell is $\frac{4}{3}\pi(H_{i+1}^3 - H_i^3)$ and for our situation this volume must be equal to V_0/ν. That is,

$$\tfrac{4}{3}\pi(H_{i+1}^3 - H_i^3) = \tfrac{4}{3}\pi(H_{max}^3 - H_{min}^3)/\nu,$$

which can be rewritten as

$$H_{i+1} = [H_i^3 + (H_{max}^3 - H_{min}^3)/\nu]^{1/3}, \quad i = 1, 2, \ldots, \nu-1. \quad (7)$$

Here the inner radius of the innermost shell (called

* Since $H = 2(\sin\theta)/\lambda = 2S$, this partitioning is equivalent to partitioning the interval $0 \le S \le S_{max}$ into ν sub-intervals.

Table 1. *Notation, definition and the theoretical expressions for the overall values of various types of R indices for truncated data*

No.	Name of index	Notation	Definition	Final expression: Earlier	Final expression: Present	Expression for local value in terms of normalized variables y_N and y_P^c
1.	Normalized conventional R index based on F	$\bar{R}_1(F_t)$	$\frac{\sum^t \lvert\lvert F_N\rvert-\lvert F_P^c\rvert/\sigma_1\rvert}{\sum^t \lvert F_N\rvert}$	$\frac{\sum_s f_s n_s [R_1(y_t)]_s}{\sum_s f_s n_s}$	$\frac{\sum_s f_s [R_1(y_t)]_s}{\sum_s f_s}$	$[R_1(y_t)]_s = \frac{\langle\lvert y_N - y_P^c\rvert\rangle_s^t}{\langle y_N\rangle_s^t}$
2.	Normalized conventional R index based on y	$\bar{R}_1(y_t)$	$\frac{\sum^t \lvert y_N - y_P^c\rvert}{\sum^t y_N}$	$\frac{\sum_s n_s [R_1(y_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R_1(y_t)]_s$	$[R_1(y_t)]_s = \frac{\langle\lvert y_N - y_P^c\rvert\rangle_s^t}{\langle y_N\rangle_s^t}$
3.	Normalized conventional R index based on I	$\bar{R}_1(I_t)$	$\frac{\sum^t \lvert I_N - I_P^c/\sigma_1^2\rvert}{\sum^t I_N}$	$\frac{\sum_s f_s^2 n_s [R_1(z_t)]_s}{\sum_s f_s^2 n_s}$	$\frac{\sum_s f_s^2 [R_1(z_t)]_s}{\sum_s f_s^2}$	$[R_1(z_t)]_s = \frac{\langle\lvert y_N^2 - (y_P^c)^2\rvert\rangle_s^t}{\langle y_N^2\rangle_s^t}$
4.	Normalized conventional R index based on z	$\bar{R}_1(z_t)$	$\frac{\sum^t \lvert z_N - z_P^c\rvert}{\sum^t z_N}$	$\frac{\sum_s n_s [R_1(z_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R_1(z_t)]_s$	$[R_1(z_t)]_s = \frac{\langle\lvert y_N^2 - (y_P^c)^2\rvert\rangle_s^t}{\langle y_N^2\rangle_s^t}$
5.	Normalized Booth-type R index based on F	${}_B\bar{R}_1(F_t)$	$\frac{\sum^t (\lvert F_N\rvert-\lvert F_P^c\rvert/\sigma_1)^2}{\sum^t \lvert F_N\rvert^2}$	$\frac{\sum_s f_s^2 n_s [{}_BR_1(y_t)]_s}{\sum_s f_s^2 n_s}$	$\frac{\sum_s f_s^2 [{}_BR_1(y_t)]_s}{\sum_s f_s^2}$	$[{}_BR_1(y_t)]_s = \frac{\langle (y_N - y_P^c)^2\rangle_s^t}{\langle y_N\rangle_s^t}$
6.	Normalized Booth-type R index based on y	${}_B\bar{R}_1(y_t)$	$\frac{\sum^t (y_N - y_p^c)^2}{\sum^t y_N^2}$	$\frac{\sum_s n_s [{}_BR_1(y_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [{}_BR_1(y_t)]_s$	$[{}_BR_1(y_t)]_s = \frac{\langle (y_N - y_P^c)^2\rangle_s^t}{\langle y_N^2\rangle_s^t}$
7.	Normalized Booth-type R index based on I	${}_B\bar{R}_1(I_t)$	$\frac{\sum^t (I_N - I_P^c/\sigma_1^2)^2}{\sum^t I_N^2}$	$\frac{\sum_s f_s^4 n_s [{}_BR_1(z_t)]_s}{\sum_s f_s^4 n_s}$	$\frac{\sum_s f_s^4 [{}_BR_1(z_t)]_s}{\sum_s f_s^4}$	$[{}_BR_1(z_t)]_s = \frac{\langle [y_N^2 - (y_P^c)^2]^2\rangle_s^t}{\langle y_N^4\rangle_s^t}$
8.	Normalized Booth-type R index based on z	${}_B\bar{R}_1(z_t)$	$\frac{\sum^t (z_n - z_P^c)^2}{\sum^t z_N^2}$	$\frac{\sum_s n_s [{}_BR_1(z_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [{}_BR_1(z_t)]_s$	$[{}_BR_1(z_t)]_s = \frac{\langle [y_N^2 - (y_P^c)^2]^2\rangle_s^t}{\langle y_N^4\rangle_s^t}$
9.	Normalized fractional-type R index based on F	$\bar{R}_1^f(F_t)$	$\frac{1}{N}\sum^t \left\lvert \frac{\lvert F_N\rvert-\lvert F_P^c\rvert/\sigma_1}{\frac{1}{2}(\lvert F_N\rvert+\lvert F_P^c\rvert/\sigma_1)} \right\rvert$	$\frac{\sum_s n_s [R_1^f(y_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R_1^f(y_t)]_s$	$[R_1^f(y_t)]_s = 2\left\langle \left\lvert \frac{y_N - y_P^c}{y_N + y_P^c} \right\rvert \right\rangle_s^t$
10.	Normalized fractional-type R index based on y	$\bar{R}_1^f(y_t)$	$\frac{1}{N}\sum^t \left\lvert \frac{y_N - y_P^c}{\frac{1}{2}(y_N + y_P^c)} \right\rvert$	$\frac{\sum_s n_s [R_1^f(y_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R_1^f(y_t)]_s$	$[R_1^f(y_t)]_s = 2\left\langle \left\lvert \frac{y_N - y_P^c}{y_N + y_P^c} \right\rvert \right\rangle_s^t$
11.	Normalized fractional-type R index based on I	$\bar{R}_1^f(I_t)$	$\frac{1}{N}\sum^t \left\lvert \frac{I_N - I_P^c/\sigma_1^2}{\frac{1}{2}(I_N + I_P^c/\sigma_1^2)} \right\rvert$	$\frac{\sum_s n_s [R_1^f(z_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R_1^f(z_t)]_s$	$[R_1^f(z_t)]_s = 2\left\langle \left\lvert \frac{y_N^2 - (y_P^c)^2}{y_N^2 + (y_P^c)^2} \right\rvert \right\rangle_s^t$
12.	Normalized fractional-type R index based on z	$\bar{R}_1^f(z_t)$	$\frac{1}{N}\sum^t \left\lvert \frac{z_N - z_P^c}{\frac{1}{2}(z_N + z_P^c)} \right\rvert$	$\frac{\sum_s n_s [R_1^f(z_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R_1^f(z_t)]_s$	$[R_1^f(z_t)]_s = 2\left\langle \left\lvert \frac{y_N^2 - (y_P^c)^2}{y_N^2 + (y_P^c)^2} \right\rvert \right\rangle_s^t$
13.	Unnormalized conventional R index based on F	$\bar{R}(F_t)$	$\frac{\sum^t \lvert\lvert F_N\rvert-\lvert F_P^c\rvert\rvert}{\sum^t \lvert F_N\rvert}$	$\frac{\sum_s f_s n_s [R(y_t)]_s}{\sum_s f_s n_s}$	$\frac{\sum_s f_s [R(y_t)]_s}{\sum_s f_s}$	$[R(y_t)]_s = \frac{\langle\lvert y_N - \sigma_1 y_P^c\rvert\rangle_s^t}{\langle y_N\rangle_s^t}$
14.	Unnormalized conventional R index based on I	$\bar{R}(I_t)$	$\frac{\sum^t \lvert I_N - I_P^c\rvert}{\sum^t I_N}$	$\frac{\sum_s f_s^2 n_s [R(z_t)]_s}{\sum_s f_s^2 n_s}$	$\frac{\sum_s f_s^2 [R(z_t)]_s}{\sum_s f_s^2}$	$[R(z_t)]_s = \frac{\langle\lvert y_N^2 - \sigma_1^2 (y_P^c)^2\rvert\rangle_s^t}{\langle y_N^2\rangle_s^t}$
15.	Unnormalized Booth-type R index based on F	${}_B\bar{R}(F_t)$	$\frac{\sum^t (\lvert F_N\rvert-\lvert F_P^c\rvert)^2}{\sum^t \lvert F_N\rvert^2}$	$\frac{\sum_s f_s^2 n_s [{}_BR(y_t)]_s}{\sum_s f_s^2 n_s}$	$\frac{\sum_s f_s^2 [{}_BR(y_t)]_s}{\sum_s f_s^2}$	$[{}_BR(y_t)]_s = \frac{\langle (y_N - \sigma_1 y_P^c)^2\rangle_s^t}{\langle y_N^2\rangle_s^t}$
16.	Unnormalized Booth-type R index based on I	${}_B\bar{R}(I_t)$	$\frac{\sum^t (I_N - I_P^c)^2}{\sum^t I_N^2}$	$\frac{\sum_s f_s^4 n_s [{}_BR(z_t)]_s}{\sum_s f_s^4 n_s}$	$\frac{\sum_s f_s^4 [{}_BR(z_t)]_s}{\sum_s f_s^4}$	$[{}_BR(z_t)]_s = \frac{\langle [y_N^2 - \sigma_1^2 (y_P^c)^2]^2\rangle_s^t}{\langle y_N^4\rangle_s^t}$
17.	Unnormalized fractional-type R index based on F	$\bar{R}^f(F_t)$	$\frac{1}{N}\sum^t \left\lvert \frac{\lvert F_N\rvert-\lvert F_P^c\rvert}{\frac{1}{2}(\lvert F_N\rvert+\lvert F_P^c\rvert)} \right\rvert$	$\frac{\sum_s n_s [R^f(y_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R^f(y_t)]_s$	$[R^f(y_t)]_s = 2\left\langle \left\lvert \frac{y_N - \sigma_1 y_P^c}{y_N + \sigma_1 y_P^c} \right\rvert \right\rangle_s^t$
18.	Unnormalized fractional-type R index based on I	$\bar{R}^f(I_t)$	$\frac{1}{N}\sum^t \left\lvert \frac{I_N - I_P^c}{\frac{1}{2}(I_N + I_P^c)} \right\rvert$	$\frac{\sum_s n_s [R^f(z_t)]_s}{\sum_s n_s}$	$(1/\nu)\sum_s [R^f(z_t)]_s$	$[R^f(z_t)]_s = 2\left\langle \left\lvert \frac{y_N^2 - \sigma_1^2 (y_P^c)^2}{y_N^2 + \sigma_1^2 (y_P^c)^2} \right\rvert \right\rangle_s^t$

Note: $\sum^t$ stands for the summation over the N observed reflections in the data. The superscript t to the summation symbol denotes that the truncated data are involved in the summation. Also note that $\bar{R}_1^f(y_t) = \bar{R}_1^f(F_t)$ and $\bar{R}_1^f(z_t) = \bar{R}_1^f(I_t)$ and hence we shall hereafter consider only $\bar{R}_1^f(F_t)$ and $\bar{R}_1^f(I_t)$.

shell 1) is given by $H_1 = H_{\min}$. $H_{\max}$ is the outer radius of the outermost (*i.e.* νth) shell.

Shifting the index from i to $i-1$, we can rewrite (7) as

$$H_i = [(H_{\max}^3 - H_{\min}^3)/\nu + H_{i-1}^3]^{1/3}, \quad i = 2, 3, \ldots, \nu \tag{8}$$

with $H_1 = H_{\min}$.

With the results of Parthasarathy & Parthasarathi (1975), the mean value of $(\sin\theta)/\lambda$ corresponding to the ith shell for which $H_{i-1} \le H \le H_i$ can be shown to be

$$\bar{H}_i = 3(H_i^4 - H_{i-1}^4)/[4(H_i^3 - H_{i-1}^3)]. \tag{9}$$

Since $H = 2(\sin\theta)/\lambda$, we can write the mean value of $(\sin\theta)/\lambda$ for the ith shell as

$$\bar{s}_i = 3(S_i^4 - S_{i-1}^4)/[4(S_i^3 - S_{i-1}^3)]. \tag{10}$$

3.2. *Atomic scattering factor of an average atom for the structure*

The atomic scattering factor f needed in the theoretical expressions for the overall value of R for any given model may be taken to be that of an average atom in the structure. Thus, if α_C, α_N and α_O are the fractional number of C, N and O atoms in the asymmetric unit then we may write

$$\bar{f} = (\alpha_C f_C^0 + \alpha_N f_N^0 + \alpha_O f_O^0) \exp[-B(\sin^2\theta)/\lambda^2], \tag{11}$$

where B is the average isotropic temperature factor for the atoms in the asymmetric unit and f_C^0, f_N^0 and f_O^0 are the atomic scattering factors of static C, N and O atoms. The quantities α_C, α_N and α_O would vary from structure to structure. However, for the purpose of obtaining convenient reference tables for use, the following strategy was used. Volumes B44 and C44 of *Acta Crystallographica* were surveyed to pick out all light-atom structures (*i.e.* structures containing* C, N and O atoms) published during 1988. If Δ_{ij} is the fractional number of atoms of type i (i is 1 for C, 2 for N and 3 for O, say) in compound j, the scattering factor $\bar{f}$ of the average atom was taken to be

$$\bar{f} = (\alpha_C f_C^0 + \alpha_N f_N^0 + \alpha_O f_O^0) \exp[-B(\sin^2\theta)/\lambda^2], \tag{12}$$

where the weights α_C, α_N and α_O are given by

$$\alpha_i = \left(\sum_{j=1}^{m} \Delta_{ij}\right) \Big/ m, \quad i = \text{C, N and O.} \tag{13}$$

Here m is the total number of compounds studied (*i.e.* 319 in the present case). The values obtained by the above procedure are $\alpha_C = 0{\cdot}739$, $\alpha_N = 0{\cdot}086$ and $\alpha_O = 0{\cdot}175$. Taking B to be 3 Å^2 we can write the scattering factor for the average atom to be

$$\bar{f} = (0{\cdot}739 f_C^0 + 0{\cdot}086 f_N^0 + 0{\cdot}175 f_O^0) \times \exp[-3(\sin^2\theta)/\lambda^2]. \tag{14}$$

The quantity $\bar{f}$ obtained in (14) was used in calculating the theoretical overall values of R indices reported in Tables 2 and 3.

3.3. *Method of computing the local value of R corresponding to given values of* $\langle|\Delta\mathbf{r}|\rangle$, σ_1^2 *and* $(\sin\theta)/\lambda$

The local value of any normalized R index is known to be a function of σ_A (see Parathasarthy & Velmurugan, 1981; Velmurugan & Parthasarathy, 1981*a*). The local value of any unnormalized R index is known to depend explicitly on σ_1 and D (Velmurugan & Parthasarathy, 1981*b*).

It is seen from the last column of Table 1 that the local value of any R index has the form

$$R = \frac{\langle g(y_N, y_P^c)\rangle_s^t}{\langle y_N^n\rangle_s^t}, \tag{15}$$

where $g(y_N, y_P^c)$ is a function of y_N and y_P^c and $n = 0$, 1, 2 and 4 as the case may be. The quantity $\langle g(y_N, y_P^c)\rangle_s^t$ for any given σ_1 and D may be evaluated from

$$\langle g(y_N, y_P^c)\rangle_s^t = \int_0^\infty \int_{y_t}^\infty g(y_N, y_P^c) P_t(y_N, y_P^c)\, dy_N\, dy_P^c, \tag{16}$$

where $P_t(y_N, y_P^c)$ is the joint p.d.f. of y_N and y_P^c for the truncated distribution. The double integral in (16) is to be evaluated numerically.*

The joint p.d.f. of y_N and y_P^c for the truncated data is known to be

$$P_t(y_N, y_P^c) = \frac{2}{\pi\sigma_B\beta_C} \exp\left[-\frac{y_N^2 + (y_P^c)^2}{2\sigma_B^2}\right] \times \cosh\left[\frac{\sigma_A y_N y_P^c}{\sigma_B^2}\right] \tag{17}$$

for situation I (Parthasarathy & Velmurugan, 1981) and

$$P_t(y_N, y_P^c) = \frac{4 y_N y_P^c}{\sigma_B^2 \beta_{NC}} \exp\left[-\frac{y_N^2 + (y_P^c)^2}{\sigma_B^2}\right] \times I_0\left[\frac{2\sigma_A y_N y_P^c}{\sigma_B^2}\right] \tag{18}$$

for situation II (Velmurugan & Parthasarathy, 1981*a*). β_C and β_{NC} are defined as

$$\beta_C = \text{erfc}\,(y_t/2^{1/2}) \tag{19}$$

* We shall neglect H atoms in our consideration.

* The numerical tables in Velmurugan & Parthasarathy (1981*a*, *b*) and Parthasarathy & Velmurugan (1981) could be used to evaluate $\langle g(y_N, y_P^c)\rangle$ using interpolation techniques. However, since the present method of directly carrying out the double integral in (16) yields more accurate results, we have evaluated $\langle g(y_N, y_P^c)\rangle$ by numerical integration.

Table 2. *Theoretical overall values of R indices* (×1000) *as a function of* $\langle|\Delta\mathbf{r}|\rangle$ (Å) *for different values of* y_t *corresponding to* $\sigma_1^2 = 1{\cdot}00$: *centrosymmetric case*

Index	y_t / $\langle\lvert\Delta\mathbf{r}\rvert\rangle$	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18	0.20	0.22	0.24	0.26	0.28	0.30	0.35	0.40
$\bar{R}_1(F_t)$	0.00	0	11	49	97	146	193	238	281	321	359	395	428	459	488	515	539	593	636
	0.15	0	46	82	126	170	212	250	286	319	350	379	406	432	455	477	497	541	576
	0.30	0	42	79	120	159	195	230	262	293	321	348	373	396	417	437	455	494	526
	0.45	0	31	74	112	148	182	215	246	275	302	327	351	372	392	411	428	464	494
	0.60	0	36	61	94	129	163	196	226	255	282	308	331	353	373	391	408	443	472
$\bar{R}_1(y_t)$	0.00	0	15	63	121	177	231	282	330	374	416	454	490	522	552	580	604	657	697
	0.15	0	51	95	148	199	245	288	327	363	397	428	456	483	507	530	550	593	626
	0.30	0	47	92	140	184	225	263	299	333	364	393	419	443	465	485	503	541	570
	0.45	0	38	87	130	171	209	246	281	313	342	370	394	417	438	456	473	508	535
	0.60	0	40	69	110	151	191	227	262	293	323	350	375	397	418	436	452	486	512
$\bar{R}_1(I_t)$	0.00	0	3	24	63	110	161	214	267	320	371	420	468	514	557	598	637	726	803
	0.15	0	55	89	136	189	244	296	346	394	439	481	522	560	596	630	662	734	795
	0.30	0	54	95	147	198	246	292	336	379	419	457	493	526	558	588	617	681	735
	0.45	0	41	102	156	202	245	287	327	365	402	437	470	501	531	559	585	644	693
	0.60	0	47	78	119	166	213	258	301	342	380	415	449	480	509	535	560	614	659
$\bar{R}_1(z_t)$	0.00	0	7	51	120	196	274	351	427	498	565	628	687	742	792	838	881	971	1042
	0.15	0	69	122	203	286	362	430	492	550	603	654	701	744	785	822	856	928	983
	0.30	0	66	138	217	283	344	404	461	515	565	612	655	695	731	764	794	856	903
	0.45	0	69	152	215	274	333	389	443	493	540	583	622	658	691	720	746	801	841
	0.60	0	59	106	178	251	315	373	425	474	518	559	595	629	658	685	709	757	793
${}_B\bar{R}_1(F_t)$	0.00	0	1	5	13	25	40	57	76	97	119	142	166	190	214	238	261	317	368
	0.15	0	2	6	15	27	40	56	73	91	111	130	151	171	191	211	231	278	321
	0.30	0	2	6	14	24	36	50	66	82	100	118	136	154	172	190	207	249	287
	0.45	0	1	6	12	22	33	46	60	75	91	108	124	141	158	174	190	228	262
	0.60	0	1	4	10	18	29	41	54	69	84	99	115	131	147	162	178	213	245
${}_B\bar{R}_1(y_t)$	0.00	0	1	10	26	47	74	104	137	172	207	244	280	315	349	382	414	483	540
	0.15	0	3	12	28	49	72	98	126	155	186	216	247	277	306	333	360	418	465
	0.30	0	3	11	25	43	64	88	114	141	168	196	223	249	275	299	321	371	411
	0.45	0	3	11	22	39	58	80	104	129	155	180	205	229	252	274	295	339	375
	0.60	0	2	8	19	35	53	73	96	119	144	168	191	214	236	257	276	317	351
${}_B\bar{R}_1(I_t)$	0.00	0	0	1	3	8	15	26	39	55	73	94	116	139	164	190	217	287	360
	0.15	0	1	4	9	17	29	43	60	79	99	121	144	168	192	217	242	305	369
	0.30	0	1	4	11	20	32	46	61	77	95	113	133	153	175	197	221	281	344
	0.45	0	1	6	13	22	31	43	56	71	88	106	125	146	167	190	213	271	329
	0.60	0	1	3	8	16	27	40	56	73	91	110	131	151	172	193	214	266	319
${}_B\bar{R}_1(z_t)$	0.00	0	0	6	24	53	94	145	202	262	326	391	456	521	585	647	706	839	948
	0.15	0	3	15	44	84	128	174	224	278	334	393	452	511	569	624	677	795	892
	0.30	0	3	22	47	75	112	156	207	262	318	375	431	486	538	588	635	738	821
	0.45	0	7	22	41	70	109	153	201	252	305	358	411	461	509	554	597	688	760
	0.60	0	3	15	43	78	115	156	200	248	297	346	394	441	485	526	564	647	711
$\bar{R}_1^f(F_t)$	0.00	0	44	140	226	298	359	411	457	498	533	565	592	617	639	658	676	711	737
	0.15	0	81	157	230	292	346	392	433	470	502	531	557	581	601	620	637	671	696
	0.30	0	66	131	195	255	309	356	398	436	469	499	525	549	570	589	605	640	665
	0.45	0	45	104	164	220	274	324	368	409	444	476	505	530	553	573	591	628	654
	0.60	0	50	88	136	189	241	291	337	380	419	455	487	515	541	564	584	625	655
$\bar{R}_1^f(I_t)$	0.00	0	80	248	390	504	597	675	740	797	845	887	924	956	984	1008	1030	1073	1104
	0.15	0	158	294	418	520	603	674	734	786	831	871	906	937	964	988	1009	1051	1082
	0.30	0	131	252	363	461	545	617	680	734	781	823	859	891	919	944	965	1009	1041
	0.45	0	89	204	312	407	493	568	634	692	743	787	826	861	891	917	940	987	1021
	0.60	0	99	173	264	355	441	518	588	650	705	754	798	836	869	899	925	977	1015

and

$$\beta_{NC} = \exp(y_t^2). \tag{20}$$

The quantity $\langle y_N^n \rangle_s^t$ may be evaluated from

$$\langle y_N^n \rangle_s^t = \int_{y_t}^{\infty} y_N^n P_t(y_N)\, dy_N, \tag{21}$$

where $P_t(y_N)$ is the probability density function of y_N for the truncated data. $P_t(y_N)$ is known to be (Ponnuswamy & Parthasarathy, 1977)

$$P_t(y_N) = (2/\pi)^{1/2} \exp(-y_N^2/2)/\beta_C \tag{22}$$

for a centrosymmetric crystal and

$$P_t(y_N) = 2y_N \exp(-y_N^2)/\beta_{NC} \tag{23}$$

for a non-centrosymmetric crystal. The integral in (21) was also evaluated numerically.

The above procedure was used to compute the theoretical overall values of the various R indices as a function of $\langle|\Delta\mathbf{r}|\rangle$ and σ_1^2 corresponding to $y_t = 0{\cdot}0$, 0·15, 0·30, 0·45 and 0·60. Since the case for which $\sigma_1^2 = 1$ (*i.e.* $P = N$) is the most useful one, the results are given in Tables 2 and 3 only for this case.* To obtain the results in Tables 2 and 3, ν and s_{max} were taken as 24 and 0·5 Å^{-1}, respectively. It may

* The tables of values corresponding to $\sigma_1^2 = 0{\cdot}1$, 0·2, 0·3, 0·4, 0·5, 0·6, 0·7, 0·8 and 0·9 have also been computed but these are not published. These can be obtained from Parthasarathy on request.

Table 3. *Theoretical overall values of R indices* (×1000) *as a function of* $\langle|\Delta\mathbf{r}|\rangle$ (Å) *for different values of* y_t *corresponding to* $\sigma_1^2 = 1{\cdot}00$: *non-centrosymmetric case*

Index	y_t / $\langle\|\Delta\mathbf{r}\|\rangle$	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18	0.20	0.22	0.24	0.26	0.28	0.30	0.35	0.40
$\bar{R}_1(F_t)$	0.00	0	2	17	45	78	111	143	174	203	231	257	281	304	325	345	363	403	434
	0.15	0	37	60	87	118	149	178	206	232	257	281	302	323	342	360	376	412	441
	0.30	0	36	61	87	114	141	168	193	217	240	262	282	301	319	335	350	384	411
	0.45	0	21	50	81	110	137	163	187	210	231	251	269	286	302	317	331	360	384
	0.60	0	35	55	75	99	123	147	171	193	213	232	250	267	283	297	310	338	361
$\bar{R}_1(y_t)$	0.00	0	2	24	59	99	138	175	209	242	272	301	327	351	373	393	411	449	479
	0.15	0	43	66	101	138	174	207	238	267	294	319	343	364	384	402	419	454	481
	0.30	0	40	69	99	132	163	194	222	249	274	298	319	340	358	375	391	423	448
	0.45	0	25	59	96	129	160	188	215	239	262	284	303	321	338	353	367	396	418
	0.60	0	40	60	85	114	143	171	197	222	244	265	284	301	317	332	345	372	393
$\bar{R}_1(I_t)$	0.00	0	0	9	33	67	105	146	188	229	269	308	346	382	416	449	480	551	611
	0.15	0	55	81	110	146	186	227	267	306	344	380	415	448	479	508	536	599	652
	0.30	0	59	86	116	152	189	226	262	298	332	366	398	428	457	485	510	569	619
	0.45	0	30	70	114	157	196	234	269	303	335	365	394	421	447	471	494	546	590
	0.60	0	48	83	110	140	173	207	241	273	304	334	362	389	414	437	459	508	549
$\bar{R}_1(z_t)$	0.00	0	1	23	71	131	194	255	314	370	423	472	519	562	602	639	672	743	798
	0.15	0	71	98	151	215	277	335	389	439	486	530	571	608	644	676	705	769	817
	0.30	0	71	108	159	216	270	322	371	418	462	503	542	578	611	642	670	729	774
	0.45	0	43	108	171	227	277	325	370	412	452	489	523	555	584	611	635	687	726
	0.60	0	70	101	144	196	247	297	342	384	422	457	489	519	546	570	592	637	671
${}_B\bar{R}_1(F_t)$	0.00	0	0	1	5	11	20	29	40	52	65	78	92	105	119	133	147	180	210
	0.15	0	1	3	8	15	23	32	43	55	67	79	92	106	119	132	145	176	204
	0.30	0	1	4	8	14	21	30	39	50	61	73	85	97	109	121	133	161	187
	0.45	0	1	3	8	13	20	28	37	47	57	68	78	89	100	111	121	147	170
	0.60	0	1	3	6	11	17	25	33	42	51	61	71	81	91	101	111	134	155
${}_B\bar{R}_1(y_t)$	0.00	0	0	4	12	24	39	56	74	94	115	136	157	178	198	218	236	277	311
	0.15	0	2	6	15	28	42	58	76	95	115	135	155	174	193	212	229	268	300
	0.30	0	2	6	14	25	38	53	70	87	106	124	142	160	178	194	210	246	275
	0.45	0	1	6	14	24	36	50	65	81	97	114	130	146	161	176	190	221	246
	0.60	0	2	5	11	20	32	45	59	74	89	104	119	134	148	161	174	202	224
${}_B\bar{R}_1(I_t)$	0.00	0	0	0	1	5	10	17	27	38	52	66	83	100	119	138	158	210	264
	0.15	0	1	3	6	11	19	28	40	54	69	86	104	122	141	160	180	231	283
	0.30	0	2	3	7	13	21	30	42	55	70	85	102	119	136	154	173	221	270
	0.45	0	1	3	9	16	24	34	45	57	70	85	100	116	132	149	166	212	258
	0.60	0	1	4	7	11	18	27	38	50	63	78	93	109	126	143	160	204	247
${}_B\bar{R}_1(z_t)$	0.00	0	0	3	16	38	68	103	143	188	236	286	336	387	436	484	530	633	719
	0.15	0	3	10	28	56	90	128	169	212	256	302	348	395	440	484	527	622	702
	0.30	0	3	11	32	57	87	121	159	201	245	291	337	382	427	470	510	601	676
	0.45	0	3	16	35	58	85	118	155	195	236	279	322	364	405	444	482	564	630
	0.60	0	4	11	27	52	82	115	151	188	227	266	305	343	380	415	448	519	576
$\bar{R}_1^f(F_t)$	0.00	0	8	52	106	157	203	244	282	315	346	373	397	419	439	457	473	505	529
	0.15	0	53	94	140	185	226	262	295	325	353	378	400	421	439	456	471	501	525
	0.30	0	46	89	129	168	205	240	271	300	327	351	373	392	410	426	441	471	493
	0.45	0	29	67	110	150	188	222	254	283	309	333	355	374	391	407	421	450	472
	0.60	0	44	70	100	133	167	201	233	263	290	315	338	359	377	394	409	440	463
$\bar{R}_1^f(I_t)$	0.00	0	16	97	195	286	367	438	500	554	603	645	683	716	746	772	795	842	876
	0.15	0	106	184	269	350	421	483	538	587	631	670	704	735	763	787	809	853	886
	0.30	0	92	176	250	321	386	446	499	547	590	629	663	693	721	745	767	811	843
	0.45	0	57	134	215	291	358	418	472	520	562	600	634	664	691	715	736	779	811
	0.60	0	88	139	197	259	321	380	435	485	529	570	605	637	666	691	714	759	793

incidentally be noted that the following results hold when $\sigma_1^2 = 1$:

$$\bar{R}(F_t) = \bar{R}_1(F_t), \qquad \bar{R}(I_t) = \bar{R}_1(I_t),$$
$${}_B\bar{R}(F_t) = {}_B\bar{R}_1(F_t), \qquad {}_B\bar{R}(I_t) = {}_B\bar{R}_1(I_t),$$
$$\bar{R}^f(F_t) = \bar{R}_1^f(F_t), \qquad \bar{R}^f(I_t) = \bar{R}_1^f(I_t).$$

Further, for any σ_1^2

$$\bar{R}_1^f(y_t) = \bar{R}_1^f(F_t), \qquad \bar{R}_1^f(z_t) = \bar{R}_1^f(I_t).$$

Hence for a complete model for which $\sigma_1^2 = 1$, we need consider only ten of the normalized indices and hence these alone are given in Tables 2 and 3.

4. Test of the theoretical results

The theoretical results in Tables 2 and 3 were tested in the case of a few models of some crystal structures. In the case of each structure two models were chosen by introducing random Gaussian errors to the positions of the atoms in the true structure. All the models chosen were of the complete type (*i.e.* $P = N$ and $\sigma_1^2 = 1$). Three of the structures chosen are centrosymmetric and three are non-centrosymmetric. The relevant details regarding the structures and the models chosen are given in Table 4. In the case of each structure the structure-factor magnitudes calculated using the coordinates of the atoms in the true structure were taken to represent their *observed* values. Using

Table 4. *Details of the structures and the models used for testing the theoretical results*

Structure	Asymmetric unit	Space group	Reference	$\langle\|\Delta\mathbf{r}\|\rangle$ (Å) Model 1	Model 2
(I)	C_6O_6	$P\bar{1}$	Kroon & Kanters (1973)	0·0459	0·1607
(II)	$C_{17}O_2$	$P2_1/c$	Geetha (personal communication)	0·0686	0·1371
(III)	$C_{12}N_2O_2$	$Pbca$	Lisgarten & Palmer (1980)	0·0846	0·1691
(IV)	$C_{16}N_6O_8$	$P1$	Kistenmacher, Hunt & Marsh (1972)	0·0971	0·1924
(V)	C_6NO_4	$P2_1$	Low, Howe, Scrimgeour & Watt (1988)	0·0684	0·1368
(VI)	$C_{21}O_3N$	$P2_12_12_1$	Sekar (personal communication)	0·0649	0·1298

Note: All the models are of the complete type (*i.e.* $P=N$, $\sigma_1^2=1$).

the coordinates of the atoms in a model, the structure-factor magnitudes of the three-dimensional reflections within the region $0\leq(\sin\theta)/\lambda\leq 0{\cdot}5$ Å^{-1} were calculated. From these two sets of structure-factor magnitudes the values of the various R indices for a particular model of a given structure were computed by using those reflections for which $y_N>0{\cdot}3$ $(=y_t)$. The R values thus obtained for the various models of the centrosymmetric structures are summarized in Table 5. Similar results for non-centrosymmetric structures are given in Table 6. The average values of $\langle|\Delta\mathbf{r}|\rangle$ obtained from the overall values of the R indices for the various models are also given in Tables 5 and 6 along with the corresponding true values. A study of Tables 5 and 6 shows that the values of $\langle|\Delta\mathbf{r}|\rangle$ estimated by the present method closely agree with the corresponding actual values of $\langle|\Delta\mathbf{r}|\rangle$.

5. Concluding remarks

(i) It may be noted here that in the theoretical derivations the crystals were taken to be triclinic. However, from the good agreement between the theoretical and experimental values in other space groups (see Tables 4 to 6), it appears that the results in Tables 2 and 3 could also be used in space groups of higher symmetry. (ii) Since it is essential to know the true value of $\langle|\Delta\mathbf{r}|\rangle$ in order to verify the theoretical results, we have used only hypothetical structures in the tests

Table 5. *Test of the theoretical results for two different models: centrosymmetric cases*

	Structure I				Structure II				Structure III			
	Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
R index	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$
$\bar{R}_1(F_t)$	9·3	0·0468	29·8	0·1636	15·1	0·0759	28·3	0·1535	17·7	0·0900	32·1	0·1800
$\bar{R}_1(y_t)$	10·7	0·0463	33·7	0·1626	16·7	0·0723	31·1	0·1471	19·6	0·0859	35·2	0·1723
${}_B\bar{R}_1(F_t)$	0·8	0·0450	8·5	0·1633	2·2	0·0760	7·7	0·1538	2·9	0·0883	9·5	0·1744
${}_B\bar{R}_1(y_t)$	1·4	0·0443	13·6	0·1563	3·3	0·0689	11·4	0·1400	4·7	0·0838	14·9	0·1659
$\bar{R}_1^f(F_t)$	15·2	0·0466	46·4	0·1770	23·9	0·0747	43·8	0·1612	28·1	0·0896	49·1	0·1947
$\bar{R}_1(I_t)$	11·5	0·0477	39·3	0·1670	19·3	0·0780	36·5	0·1535	21·0	0·0850	39·2	0·1665
$\bar{R}_1(z_t)$	15·9	0·0453	51·0	0·1581	25·4	0·0712	47·1	0·1437	29·4	0·0836	53·4	0·1676
${}_B\bar{R}_1(I_t)$	0·6	0·0457	8·7	0·1711	1·8	0·0756	6·8	0·1488	1·2	0·0622	4·5	0·1186
${}_B\bar{R}_1(z_t)$	2·1	0·0389	23·2	0·1491	5·7	0·0671	19·8	0·1365	7·7	0·0811	27·0	0·1629
$\bar{R}_1^f(I_t)$	28·8	0·0465	76·8	0·1745	43·6	0·0749	73·1	0·1589	50·0	0·0893	80·5	0·1914
$\langle\|\Delta\mathbf{r}\|\rangle_{\text{est}}$		0·0453		0·1643		0·0735		0·1497		0·0839		0·1694
$\langle\|\Delta\mathbf{r}\|\rangle_{\text{true}}$		0·0459		0·1607		0·0686		0·1371		0·0846		0·1691

Note: R is in % and $\langle|\Delta\mathbf{r}|\rangle$ is in Å. $\langle|\Delta\mathbf{r}|\rangle_{\text{est}}$ is the average value in the respective columns.

Table 6. *Test of the theoretical results for two different models: non-centrosymmetric cases*

	Structure IV				Structure V				Structure VI			
	Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
R index	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$	$\bar{R}$	$\langle\|\Delta\mathbf{r}\|\rangle$
$\bar{R}_1(F_t)$	14·9	0·1059	27·6	0·2140	9·9	0·0689	18·5	0·1336	10·5	0·0733	20·5	0·1500
$\bar{R}_1(y_t)$	17·0	0·1045	30·7	0·2086	11·5	0·0697	21·0	0·1314	11·6	0·0703	22·7	0·1437
${}_B\bar{R}_1(F_t)$	2·2	0·1022	8·0	0·2117	1·0	0·0667	3·4	0·1289	1·1	0·0700	4·1	0·1436
${}_B\bar{R}_1(y_t)$	3·9	0·1013	12·9	0·2056	1·9	0·0691	6·0	0·1282	1·7	0·0655	6·5	0·1341
$\bar{R}_1^f(F_t)$	21·2	0·1040	35·0	0·1992	14·7	0·0692	25·3	0·1284	14·7	0·0692	28·4	0·1490
$\bar{R}_1(I_t)$	20·2	0·1070	40·0	0·2213	13·0	0·0678	25·8	0·1378	14·2	0·0744	28·0	0·1500
$\bar{R}_1(z_t)$	28·2	0·1046	53·2	0·2149	18·7	0·0698	35·3	0·1327	18·8	0·0702	36·9	0·1392
${}_B\bar{R}_1(I_t)$	2·1	0·1000	9·1	0·2071	0·8	0·0633	3·2	0·1233	0·8	0·0633	3·2	0·1233
${}_B\bar{R}_1(z_t)$	8·4	0·0980	30·9	0·2078	3·7	0·0640	13·1	0·1253	3·3	0·0608	13·0	0·1247
$\bar{R}_1^f(I_t)$	39·7	0·1037	63·3	0·2024	28·1	0·0687	46·7	0·1279	28·6	0·0701	52·1	0·1492
$\langle\|\Delta\mathbf{r}\|\rangle_{\text{est}}$		0·1031		0·2092		0·0677		0·1297		0·0687		0·1407
$\langle\|\Delta\mathbf{r}\|\rangle_{\text{true}}$		0·0971		0·1924		0·0684		0·1368		0·0649		0·1298

Note: See note to Table 5 for details.

described in § 4. In such hypothetical cases, $|F_N|$ will be free from errors of observation. However, when one uses the observed overall value of an R index for finding $\langle|\Delta\mathbf{r}|\rangle$, one must remember that the experimental errors in $|F_{obs}|$ would also contribute to the overall value of the R index. Owing to this one has to note the following two points in estimating $\langle|\Delta\mathbf{r}|\rangle$ in actual cases. (*a*) Since the overall values of Booth-type indices for a complete model (*i.e.* $P = N$) are generally small, they would not be suitable for estimating the mean coordinate error of a complete model. (*b*) The $\langle|\Delta\mathbf{r}|\rangle$ value obtained for a model from the observed overall values of R indices may be somewhat overestimated.

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The Minimum Probable Values of Residuals for the Best Centrosymmetric Model of an Approximately Centrosymmetric Crystal

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Abstract

Theoretically expected overall values of ten types of normalized R indices are derived for the best centrosymmetric model of a non-centrosymmetric crystal which is approximately centrosymmetric as a function of the mean coordinate error $\langle|\Delta\mathbf{r}|\rangle$ of the best centrosymmetric model of the non-centrosymmetric crystal. The results obtained were tested in a few cases.

1. Introduction

The joint probability density function of the normalized structure-factor magnitude y_N of a non-centrosymmetric crystal which is approximately centrosymmetric and that (*i.e.* y_N^c) calculated for the best centrosymmetric model (see later for an explanation of this nomenclature) has been worked out by Swaminathan & Srinivasan (1975) (SS, 1975). They have used this distribution to obtain the *local value* of the normalized Booth-type index ${}_BR_1(y_N)$ (see Table 1 for a definition) as a function of a parameter D [see equation (12) for a definiton of D]. A number of other R indices which are more efficient in the refinement stage are available in the literature [see Elango & Parthasarathy (1990) for their definitions and notation] and it is worthwhile to obtain the theoretical expressions for their overall values for the present situation. From a practical point of view, the overall value finds more general use than the local values of R indices. Further, it is essential to take into account the effect of data truncation due to unobserved reflections into the theoretical treatment. We shall therefore derive the theoretical expressions for the *overall values* of different types of R indices and use them to obtain the overall values of R indices *directly* as a function of $\langle|\Delta\mathbf{r}|\rangle$ in the form of a table. In this paper we shall follow the notation and nomenclature used by Elango & Parthasarathy (1990). We

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