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Theoretical Evaluation of the Overall Values of Discrepancy Indices for Truncated Data. I. Normalized *R* indices for a Centrosymmetric Crystal with Similar Atoms

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Abstract

Theoretical expressions for the local values of six types of normalized *R* indices applicable to truncated data are derived for a centrosymmetric crystal by taking the model structure to be of the imperfectly related incomplete type. These indices are tabulated as functions of σ_A and y_t. These results can be used to obtain the overall values of the *R* indices applicable to truncated data which is characterized by a given value of y_t.

1. Introduction

Values of different types of discrepancy indices (*i.e. R* indices) have been worked out in the literature for a number of crystallographic situations, such as crystals with similar atoms, crystals with heavy atoms, crystals with pseudo-symmetry in the atomic distribution, *etc.* (for details see Srinivasan & Parthasarathy, 1976, and the review of Parthasarathy, 1975). These results were obtained under the assumption that all the independent reflections in a given range of $(\sin\theta/\lambda)$ (*e.g.* Cu $K\alpha$ sphere) are available in the data. However, in actual crystals, the observed intensity of a certain percentage of reflections may be negative and many crystallographers truncate the data sets by omitting such reflections as well as those whose net counts are less than one to two times the standard deviation of this value (Stout & Jensen, 1968). Hence, it would be useful to evaluate theoretically the overall values of the various *R* indices applicable to such *truncated* data, wherein the reflections for which $y_N < y_t$ $(=\sqrt{z_t})$ are omitted.† In this series of papers we shall therefore derive the theoretical expressions of the various *R* indices corresponding to different crystallographic situations and show how these results could be used to compute their theoretical *overall values*. Since the various indices behave differently under different situations (Parthasarathy & Parthasarathi, 1975; Parthasarathi & Parthasarathy, 1977; PP, 1977 hereafter), we shall deal with all the *R* indices in this series.

In this series we shall mostly follow the notations used in chapters 5 and 6 of Srinivasan & Parthasarathy (1976; hereafter SP, 1976). We shall use the abbreviations *C* and *NC* to denote the centrosymmetric and non-centrosymmetric cases respectively. We shall denote the joint probability density function (joint p.d.f. hereafter) of the normalized structure amplitudes y_N and y_P^c valid for the complete data by $P(y_N,y_P^c)$ and that valid for the truncated data by $P_t(y_N,y_P^c)$. For convenience we shall refer to $P_t(y_N,y_P^c)$ as the truncated distribution function. The expectation value of $f(y_N,y_P^c)$ for the truncated data will be denoted by $\langle f(y_N,y_P^c)\rangle_t$ and that for the complete data by $\langle f(y_N,y_P^c)\rangle$.

The experimental value of an *R* index is usually computed by taking all the independent observed reflections as a single group. We refer to the value of the *R* index thus obtained as the *overall value* of the *R* index. A number of factors, such as the positional errors in the atoms in the model, lack of similarity of the atoms in the unit cell, *etc.*, cause the value of an *R* index for a general model to vary with $\sin\theta/\lambda$. The theoretical evaluation of the overall value of an *R* index is therefore generally carried out in two stages; namely, (i) evaluation of the *R* index in different narrow regions of $\sin\theta/\lambda$ (within which the atomic scattering factors can be treated as constant) and (ii) evaluation of the overall value by taking care of the factors which change with $\sin\theta/\lambda$ (*e.g.* atomic scattering factors) and by giving proper weights depending on the number of observed reflections in the various ranges. We shall therefore refer to the value of an *R* index calculated using reflections in a narrow range of $\sin\theta/\lambda$ as a *local value* of the *R* index in order to distinguish it from its overall value. The overall value of an *R* index will be

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† For convenience, we shall refer to the data which consist of all the theoretically possible independent reflections within a given region of $(\sin\theta/\lambda)$ as the *complete data* and the data which exclude the reflections for which $y_N < y_t$ as the *truncated data*.

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denoted with a bar over the corresponding symbol, while the local value of the index will be denoted without the bar.

In this paper we shall obtain, for a centrosymmetric crystal, the theoretical expressions for the local values of the six normalized R indices,* *viz.* $R_1(F)$, $R_1(I)$, ${}_BR_1(F)$, ${}_BR_1(I)$, $R_1^f(F)$ and $R_1^f(I)$ and show how these could be used to evaluate the overall values of these indices.

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

2.1. *Preliminary results*

We shall presently explain the general notation and nomenclature regarding the overall values of different types of R indices computed for truncated data by taking the conventional normalized index $R_1(F)$ as an illustrative example. The corresponding results for the other indices can be similarly obtained.

The overall value of the conventional normalized index $R_1(F)$ applicable to the complete data is defined to be (SP, 1976)

$$\bar{R}_1(F) = \frac{\sum_{hkl} ||F_N| - |F_P^c|/\sigma_1|}{\sum_{hkl} |F_N|}, \tag{1}$$

where the summation is over *all* the theoretically possible independent reflections within a given (sin θ/λ) range† ($0 \le s \le S_{\max}$, say), $|F_P^c|$ is the magnitude of the calculated structure factor of the trial structure consisting of P out of N atoms in the unit cell and $|F_N|$ is the magnitude of the structure factor of the crystal structure. Here σ_1^2 is defined to be‡

$$\sigma_1^2 = \langle |F_P^c|^2 \rangle / \langle |F_N|^2 \rangle = \sigma_P^2/\sigma_N^2. \tag{2}$$

For a structure with similar atoms

$$\sigma_1^2 = P/N, \tag{3}$$

which is a constant independent of sin θ/λ. The overall value of this index computed with the truncated data is denoted by $[\bar{R}_1(F)]_t$ and is defined to be

$$[\bar{R}_1(F)]_t = \frac{\sum_{hkl}^t ||F_N| - |F_P^c|/\sigma_1|}{\sum_{hkl}^t |F_N|}, \tag{4}$$

where $\sum_{hkl}^t$ means that the summation is over the independent reflections of the *truncated* data in the range 0 to $S_{\max}$. In our theoretical studies, it is convenient to use the normalized variables y_N and y_P^c defined by

$$y_N = |F_N|/\sigma_N, \; y_P^c = |F_P^c|/\sigma_P. \tag{5}$$

Making use of (5), we can rewrite (4) as

$$[\bar{R}_1(F)]_t = \frac{\sum_{hkl}^t \sigma_N |y_N - y_P^c|}{\sum_{hkl}^t \sigma_N y_N}. \tag{6}$$

If the reflections are divided into groups based on the values of s, we can rewrite (6) as

$$[\bar{R}_1(F)]_t = \frac{\sum_s \sum_r^t \sigma_{Nsr} |y_N - y_P^c|_{sr}}{\sum_s \sum_r^t \sigma_{Nsr} y_{Nsr}}, \tag{7}$$

where the summation over r is carried out over the reflections in a given range of sin θ/λ and over s is carried out over the various ranges into which the inverval 0 to $S_{\max}$ has been partitioned. Here σ_{Nsr} denotes the value of σ_N for reflection r in the range s. If the sin θ/λ ranges are sufficiently narrow, we can take the values of σ_{Nsr} for the different reflections in the range s to be the same (σ_{Ns}, say). We can therefore rewrite (7) as

$$[\bar{R}_1(F)]_t = \frac{\sum_s \sigma_{Ns} \sum_r^t |y_N - y_P^c|_{sr}}{\sum_s \sigma_{Ns} \sum_r^t y_{Nsr}}, \tag{8}$$

If n_s is the number of *observed* independent reflections in the range s in the truncated data we can write (8) as

$$[\bar{R}_1(F)]_t = \frac{\sum_s \sigma_{Ns} n_s [\langle |y_N - y_P^c| \rangle_s]_t}{\sum_s \sigma_{Ns} n_s [\langle y_N \rangle_s]_t}, \tag{9}$$

where $[\langle |y_N - y_P^c| \rangle_s]_t$ and $[\langle y_N \rangle_s]_t$ denote respectively the expectation values of $|y_N - y_P^c|$ and y_N for the observed reflections in the range s of the truncated data.

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* We shall not consider the indices $R_1^*(F)$ and $R_1^*(I)$ since $R_1^f(F)$ and $R_1^f(I)$ are somewhat better than the former two (PP, 1977).

† We shall use s to stand for sin θ/λ. $S_{\max}$ is the maximum value of s for the given data.

‡ We shall denote $1 - \sigma_1^2$ by σ_2^2.

Table 1. *Definition of the overall values of various normalized R indices for truncated data and related results*

Number	Name of the R index	Notation for the overall value of the index	Overall value of the index: Definition*	Overall value of the index: Equivalent expression	Definition of the local value of the unnormalized indices based on the normalized variables y_N and y_P^c	
1	Conventional index based on F	$[\bar{R}_1(F)]_t$	$\dfrac{\sum^t \lvert\lvert F_N\rvert - \lvert F_P^c\rvert/\sigma_1\rvert}{\sum^t \lvert F_N\rvert}$	$\dfrac{\sum_s f_s\, n_s [R_1(y)]_t}{\sum_s f_s\, n_s}$	$[R_1(y)]_t$	$= \dfrac{\langle \lvert y_N - y_P^c\rvert\rangle_t}{\langle y_N\rangle_t}$
2	Conventional index based on I	$[\bar{R}_1(I)]_t$	$\dfrac{\sum^t \lvert I_N - I_P^c/\sigma_1^2\rvert}{\sum^t I_N}$	$\dfrac{\sum_s f_s^2\, n_s [R_1(z)]_t}{\sum_s f_s^2\, n_s}$	$[R_1(z)]_t$	$= \dfrac{\langle \lvert y_N^2 - (y_P^c)^2\rvert\rangle_t}{\langle y_N^2\rangle_t}$
3	Booth-type index based on F	$[{}_B\bar{R}_1(F)]_t$	$\dfrac{\sum^t (\lvert F_N\rvert - \lvert F_P^c\rvert/\sigma_1)^2}{\sum^t \lvert F_N\rvert^2}$	$\dfrac{\sum_s f_s^2\, n_s [{}_BR_1(y)]_t}{\sum_s f_s^2\, n_s}$	$[{}_BR_1(y)]_t$	$= \dfrac{\langle (y_N - y_P^c)^2\rangle_t}{\langle y_N^2\rangle_t}$
4	Booth-type index based on I	$[{}_B\bar{R}_1(I)]_t$	$\dfrac{\sum^t (I_N - I_P^c/\sigma_1^2)^2}{\sum^t I_N^2}$	$\dfrac{\sum_s f_s^4\, n_s [{}_BR_1(z)]_t}{\sum_s f_s^4\, n_s}$	$[{}_BR_1(z)]_t$	$= \dfrac{\langle (y_N^2 - (y_P^c)^2)^2\rangle_t}{\langle y_N^4\rangle_t}$
5	Fractional-type index based on F	$[\bar{R}_1^f(F)]_t$	$\dfrac{1}{N_0}\sum^t \left\lvert \dfrac{\lvert F_N\rvert - \lvert F_P^c\rvert/\sigma_1}{(\lvert F_N\rvert + \lvert F_P^c\rvert/\sigma_1)/2} \right\rvert$	$\dfrac{\sum_s n_s [R_1^f(y)]_t}{\sum_s n_s}$	$[R_1^f(y)]_t$	$= 2\left\langle \left\lvert \dfrac{y_N - y_P^c}{y_N + y_P^c} \right\rvert \right\rangle_t$
6	Fractional-type index based on I	$[\bar{R}_1^f(I)]_t$	$\dfrac{1}{N_0}\sum^t \left\lvert \dfrac{I_N - I_P^c/\sigma_1^2}{(I_N + I_P^c/\sigma_1^2)/2} \right\rvert$	$\dfrac{\sum_s n_s [R_1^f(z)]_t}{\sum_s n_s}$	$[R_1^f(z)]_t$	$= 2\left\langle \left\lvert \dfrac{y_N^2 - (y_P^c)^2}{y_N^2 + (y_P^c)^2} \right\rvert \right\rangle_t$

* The summation $\sum^t$ is over the independent reflections of the truncated data. The summation $\sum_s$ is over the different narrow ranges of $\sin\theta/\lambda_0$. N_0 is the number of reflections in the truncated data.

Since $[\langle y_N\rangle_s]_t$ is a property of the structure but not of the model and since for a structure with similar atoms† the p.d.f. of y_N is independent of s (Wilson, 1949), it follows that $[\langle y_N\rangle_s]_t$ will depend only on y_t. Hence we can write $[\langle y_N\rangle_s]_t$ simply as $[\langle y_N\rangle]_t$. We can therefore rewrite (9) as

$$[\bar{R}_1(F)]_t = \frac{\sum_s n_s\, \sigma_{Ns} [R_1(y)]_t}{\sum_s n_s\, \sigma_{Ns}}, \qquad (10)$$

where $[R_1(y)]_t$ is defined to be

$$[R_1(y)]_t = \frac{[\langle \lvert y_N - y_P^c\rvert\rangle_s]_t}{[\langle y_N\rangle]_t}. \qquad (11)$$

We refer to $[R_1(y)]_t$ as the local value of $R_1(y)$ calculated with the *observed* reflections in a particular range s. For equal-atom atructures, $\sigma_N = \sqrt{Nf}$. We can therefore rewrite (9) as

$$[\bar{R}_1(F)]_t = \frac{\sum_s f_s\, n_s [R_1(y)]_t}{\sum_s f_s\, n_s}. \qquad (12)$$

* For a structure with heavy atoms the p.d.f. of y_N involves the parameter σ_1^2. Since σ_1^2 is a function of s, it follows that $\lvert\langle y_N\rangle_s\rvert_t$ could also depend on s.

It is clear from (12) that we can evaluate the overall value $[\bar{R}_1(F)]_t$ for the truncated data in $0 \le s < S_{\max}$ if we know, corresponding to the various ranges of s, the values of the scattering factor of the atom, the number of independent reflections in the truncated data and the local values of $[R_1(y)]_t$. Of these, f_s and n_s for a given crystal are known quantities; we shall show in the rest of this paper how the local values $[R_1(y)]_t$ and those for the other normalized R indices can be obtained theoretically.

As stated earlier, the above considerations can be carried over to the other five normalized R indices. The final expressions which are the analogues of (12) are hence listed in Table 1 without derivation.

2.2. *Derivation of the joint p.d.f. of y_N and y_P^c for the truncated data*

It is seen from columns 5 and 6 of Table 1 that the overall values of the various normalized R indices can be calculated if we obtain the expectation values of simple functions of y_N and y_P^c. Thus the overall values of these R indices can, in principle, be evaluated if we know the joint p.d.f. of y_N and y_P^c for the truncated data, *i.e.* the function $P_t(y_N, y_P^c)$. It is clear that the function

$P_t(y_N,y_P^c)$ is related to the function $P(y_N,y_P^c)$ by

$$P_t(y_N,y_P^c)=\frac{1}{\beta}P(y_N,y_P^c),\quad y_t\le y_N<\infty \qquad (13)$$
$$0\le y_P^c<\infty,$$

where β* is given by

$$\beta=\int_{y_t}^{\infty}\int_{0}^{\infty}P(y_N,y_P^c)\,dy_N dy_P^c. \qquad (14)$$

The function $P(y_N,y_P^c)$ for the C case is known to be (SP, 1976)

$$P(y_N,y_P^c)=\frac{2}{\pi\sigma_B}\exp\left\{-\frac{[y_N^2+(y_P^c)^2]}{2\sigma_B^2}\right\}\times\cosh\left[\frac{\sigma_A y_N y_P^c}{\sigma_B^2}\right],$$
$$0\le y_N<\infty,\qquad 0\le y_P^c<\infty, \qquad (15)$$

where

$$\sigma_A^2+\sigma_B^2=1,\qquad \sigma_A=\sigma_1 D \qquad (16)$$

$$D=\exp\left(-\frac{\pi^3}{4}|H|^2\langle|\Delta r|\rangle^2\right),\ |H|=2s. \qquad (17)$$

Making use of (15) and (16), we have shown {in the Appendix† [see (A-10)]} that β_C is given by

$$\beta_C=\operatorname{erfc}(y_t/\sqrt{2}). \qquad (18)$$

From (13) and (15), we obtain

$$P_t(y_N,y_P^c)=\frac{2}{\beta_C\pi\sigma_B}\exp\left\{-\frac{[y_N^2+(y_P^c)^2]}{2\sigma_B^2}\right\}\times\cosh\left[\frac{\sigma_A y_N y_P^c}{\sigma_B^2}\right],$$
$$y_t\le y_N<\infty,\qquad 0\le y_P^c<\infty. \qquad (19)$$

2.3. *Derivation of the theoretical expressions for the local values of normalized R indices applicable to truncated data*

Index $[R_1(y)]_t$. From the definition of $[R_1(y)]_t$ in Table 1, we have

$$[R_1(y)]_t=\frac{1}{\langle y_N\rangle_t}\int_{y_t}^{\infty}\int_{0}^{\infty}|y_N-y_P^c|\,P_t(y_N,y_P^c)\,dy_N\,dy_P^c, \qquad (20)$$

where $P_t(y_N,y_P^c)$ is given by (19). Making use of (13), we can rewrite (20) as

$$[R_1(y)]_t=\frac{\langle y_N\rangle}{\beta_C\langle y_N\rangle_t}\left[\frac{1}{\langle y_N\rangle}\int_0^{\infty}\int_0^{\infty}|y_N-y_P^c|\,P(y_N,y_P^c)\times dy_N\,dy_P^c-\frac{1}{\langle y_N\rangle}\int_0^{y_t}\int_0^{\infty}|y_N-y_P^c|\times P(y_N,y_P^c)\,dy_N\,dy_P^c\right]. \qquad (21)$$

The first term within the square brackets in (21) represents $\langle|y_N-y_P^c|\rangle/\langle y_N\rangle$, which by definition is $R_1(y)$. It has been shown that (SP, 1976)

$$R_1(y)=[2(1+\sigma_A)]^{1/2}+[2(1-\sigma_A)]^{1/2}-2. \qquad (22)$$

Making use of the known result that $\langle y_N\rangle=\sqrt{2/\pi}$ (Wilson, 1949) and the expressions for β_C [see (18)] and $\langle y_N\rangle_t$ [see (A-11)], we can rewrite (21) as

$$[R_1(y)]_t=\exp(y_t^2/2)\left[R_1(y)-\sqrt{\frac{\pi}{2}}\int_0^{y_t}\int_0^{\infty}|y_N-y_P^c|\times P(y_N,y_P^c)\,dy_N\,dy_P^c\right]. \qquad (23)$$

It is convenient to change the variables of integration to u and v where

$$u=y_N/(1+y_N)\quad\text{and}\quad v=y_P^c/(1+y_P^c). \qquad (24)$$

Thus, we obtain

$$[R_1(y)]_t=\exp(y_t^2/2)\left[R_1(y)-\sqrt{\frac{\pi}{2}}\int_0^{y_t/(1+y_t)}\int_0^{1}\left|\frac{u}{1-u}-\frac{v}{1-v}\right|\times P\left(\frac{u}{1-u},\frac{v}{1-v}\right)\times\frac{du}{(1-u)^2}\frac{dv}{(1-v)^2}\right]. \qquad (25)$$

Here, $P[u/(1-u),v/(1-v)]$ means that in expression (15) for $P(y_N,y_P^c)$, y_N is to be replaced by $u/(1-u)$ and y_P^c by $v/(1-v)$.

Index $[R_1(z)]_t$. From the definition of $[R_1(z)]_t$ in Table 1 we have

$$[R_1(z)]_t=\frac{1}{\langle y_N^2\rangle_t}\int_{y_t}^{\infty}\int_{0}^{\infty}|y_N^2-(y_P^c)^2|\,P_t(y_N,y_P^c)\,dy_N\,dy_P^c. \qquad (26)$$

Following the method used for $[R_1(y)]_t$ and using (A-13) and the definition (see SP, 1976)

$$R_1(z)=\langle|z_N-z_P^c|\rangle=\langle|y_N^2-(y_P^c)^2|\rangle,$$

* Since the function $P(y_N,y_P^c)$ for the C and NC cases is different, β will be different for the two cases. Hence, the quantity appropriate to the C and NC cases will be denoted by β_C and β_{NC} respectively.

† This appendix has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35848 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

we can rewrite (26) as

$$[R_1(z)]_t = \left[R_1(z) - \int_0^{y_t} \int_0^{\infty} |y_N^2 - (y_P^c)^2| \times P(y_N, y_p^c)\, dy_N\, dy_P^c \right] \times [\beta_C + \sqrt{(2/\pi)}\, y_t \exp(-y_t^2/2)]^{-1}. \quad (27)$$

It is known that (SP, 1976)

$$R_1(z) = \frac{4}{\pi}\sigma_B. \quad (28)$$

Making use of the substitution (24), we can rewrite (27) as

$$[R_1(z)]_t = \left[R_1(z) - \int_0^{y_t/(1+y_t)} \int_0^1 \left| \left(\frac{u}{1-u}\right)^2 - \left(\frac{v}{1-v}\right)^2 \right| P\left(\frac{u}{1-u}, \frac{v}{1-v}\right) \times \frac{du}{(1-u)^2} \frac{dv}{(1-v)^2} \right] \times [\beta_C + \sqrt{(2/\pi)}\, y_t \exp(-y_t^2/2)]^{-1}. \quad (29)$$

Index $[{}_BR_1(y)]_t$. From the definition of $[{}_BR_1(y)]_t$ given in Table 1 we can obtain

$$[{}_BR_1(y)]_t = \frac{\langle y_N^2\rangle_t + \langle (y_P^c)^2\rangle_t - 2\langle y_N y_P^c\rangle_t}{\langle y_N^2\rangle_t}. \quad (30)$$

Substituting for $\langle y_N^2\rangle_t$, $\langle (y_P^c)^2\rangle_t$ and $\langle y_N y_P^c\rangle_t$ from (*A*-13), (*A*-18) and (*A*-23) respectively and simplifying the result with (16), we obtain

$$[{}_BR_1(y)]_t = \left[{}_BR_1(y) + 2(\beta_C - 1) + \sqrt{(2/\pi)}\, y_t(1+\sigma_A^2)\exp(-v_t^2/2) - \frac{4}{\pi}\left\{ \sigma_B^3[\exp(-y_t^2/2\sigma_B^2) - 1] - \sigma_A\sqrt{\pi}\int_0^{y_t^2/2} \sqrt{u}\exp(-u) \times \operatorname{erf}\left(\frac{\sigma_A}{\sigma_B}\sqrt{u}\right) du \right\} \right] \times [\beta_C + \sqrt{(2/\pi)}\, y_t \exp(-y_t^2/2)]^{-1}. \quad (31)$$

${}_BR_1(y)$ in (31) is given by (SP, 1976)

$${}_BR_1(y) = \langle (y_N - y_P^c)^2\rangle / \langle y_N^2\rangle = \langle (y_N - y_P^c)^2\rangle = 2 - \frac{4}{\pi}[\sigma_B + \sigma_A \sin^{-1}(\sigma_A)]. \quad (32)$$

Index $[{}_BR_1(z)]_t$. From the definition of $[{}_BR_1(z)]_t$ given in Table 1 we can write

$$[{}_BR_1(z)]_t = \frac{\langle y_N^4\rangle_t + \langle (y_P^c)^4\rangle_t - 2\langle y_N^2 (y_P^c)^2\rangle_t}{\langle y_N^4\rangle_t}. \quad (33)$$

Substituting for $\langle y_N^4\rangle_t$, $\langle (y_P^c)^4\rangle_t$ and $\langle y_N^2 (y_P^c)^2\rangle_t$ from (*A*-15), (*A*-22) and (*A*-24) respectively and simplifying, we obtain

$$[{}_BR_1(z)]_t = \{ {}_BR_1(z) + \sqrt{(2/\pi)}(1-\sigma_A^2)(y_t/3\beta_C) \times \exp(-y_t^2/2)[(1+y_t^2) + \sigma_A^2(3-y_t^2)]\} [1 + \sqrt{(2/\pi)}(y_t/3\beta_C) \times (3+y_t^2)\exp(-y_t^2/2)]^{-1}. \quad (34)$$

In obtaining (34) we have used (16) as well as the result (SP, 1976)

$${}_BR_1(z) = \tfrac{4}{3}\sigma_B^2. \quad (35)$$

Index $[R_1^f(y)]_t$. From the definition of $[R_1^f(y)]_t$ given in Table 1, we can write

$$[R_1^f(y)]_t = 2\int_{y_t}^{\infty}\int_0^{\infty} \left| \frac{y_N - y_P^c}{y_N + y_P^c} \right| P_t(y_N, y_P^c)\, dy_N\, dy_P^c. \quad (36)$$

With (13) we can rewrite (36) as

$$[R_1^f(y)]_t = \frac{1}{\beta_C}\left[2\int_0^{\infty}\int_0^{\infty} \left| \frac{y_N - y_P^c}{y_N + y_P^c} \right| P(y_N, y_P^c)\, dy_N\, dy_P^c - 2\int_0^{y_t}\int_0^{\infty} \left| \frac{y_N - y_P^c}{y_N + y_P^c} \right| \times P(y_N, y_P^c)\, dy_N\, dy_P^c \right]. \quad (37)$$

The first term within the square brackets represents $R_1^f(y)$ (see PP, 1977). Making use of the transformation (24) in the integrals occurring as the second term on the right-hand side of (37), we obtain

$$[R_1^f(y)]_t = \frac{1}{\beta_C}\left[R_1^f(y) - 2\int_0^{y_t/(1+y_t)}\int_0^1 \left| \left(\frac{u}{1-u} - \frac{v}{1-v}\right) \Big/ \left(\frac{u}{1-u} + \frac{v}{1-v}\right) \right| \times P\left(\frac{u}{1-u}, \frac{v}{1-v}\right) \times \frac{du}{(1-u)^2}\frac{dv}{(1-v)^2} \right]. \quad (38)$$

$R_1^f(y)$ has been shown to be (PP, 1977)

$$R_1^f(y) = \frac{2}{\pi}\{[(1+\sigma_A)/(1-\sigma_A)]^{1/2} \ln [2/(1+\sigma_A)] - [(1-\sigma_A)/(1+\sigma_A)]^{1/2} \ln [2/(1-\sigma_A]\}. \quad (39)$$

Index $[R_1^f(z)]_t$. From the definition of $[R_1^f(z)]_t$ given in Table 1 we can write

$$[R_1^f(z)]_t = 2\int_{y_t}^{\infty}\int_{0}^{\infty}\left|\frac{y_N^2-(y_P^c)^2}{y_N^2+(y_P^c)^2}\right| P_t(y_N, y_p^c)\, dy_N\, dy_P^c. \quad (40)$$

Following the same procedure as that used for $[R_1^f(y)]_t$ we can show that (40) becomes

$$[R_1^f(z)]_t = \frac{1}{\beta_C}\left[R_1^f(z) - 2\int_0^{y_t/(1+y_t)}\int_0^1 \left|\left[\left(\frac{u}{1-u}\right)^2 - \left(\frac{v}{1-v}\right)^2\right] \Big/ \left[\left(\frac{u}{1-u}\right)^2 + \left(\frac{v}{1-v}\right)^2\right]\right| P\left(\frac{u}{1-u}, \frac{v}{1-v}\right) \times \frac{du}{(1-u)^2}\frac{dv}{(1-v)^2}\right], \quad (41)$$

Table 2. *Values of* $[R_1(y)]_t$ *and* $[R_1(z)]_t$ *as functions of* σ_A *and* y_t *for the centrosymmetric case*

	$[R_1(y)]_t$					$[R_1(z)]_t$				
σ_A ↓ y_t →	0.00	0.15	0.30	0.45	0.60	0.00	0.15	0.30	0.45	0.60
0.000	82.843	72.763	65.864	61.396	58.779	127.324	115.581	105.008	96.268	89.576
0.040	82.796	72.715	65.823	61.360	58.745	127.222	115.498	104.942	96.217	89.535
0.080	82.616	72.571	65.701	61.253	58.646	126.916	115.249	104.744	96.061	89.410
0.120	82.331	72.331	65.497	61.074	58.479	126.404	114.831	104.412	95.800	89.201
0.160	81.930	71.993	65.209	60.821	58.243	125.684	114.243	103.945	95.432	88.903
0.200	81.410	71.554	64.835	60.492	57.936	124.751	113.481	103.337	94.951	88.515
0.240	80.768	71.012	64.373	60.085	57.555	123.603	112.539	102.584	94.354	88.029
0.280	80.000	70.363	63.819	59.596	57.096	122.231	111.413	101.681	93.634	87.440
0.320	79.100	69.602	63.169	59.021	56.556	120.629	110.094	100.619	92.783	86.740
0.360	78.061	68.723	62.417	58.355	55.928	118.787	108.573	99.389	91.791	85.917
0.400	76.876	67.720	61.557	57.591	55.205	116.694	106.838	97.980	90.646	84.960
0.420	76.226	67.169	61.085	57.169	54.806	115.550	105.887	97.203	90.013	84.427
0.440	75.536	66.583	60.582	56.721	54.379	114.337	104.876	96.377	89.335	83.854
0.460	74.803	65.962	60.047	56.243	53.924	113.053	103.805	95.497	88.611	83.240
0.480	74.027	65.303	59.480	55.735	53.440	111.697	102.670	94.563	87.839	82.581
0.500	73.205	64.605	58.878	55.195	52.923	110.266	101.469	93.571	87.015	81.874
0.520	72.336	63.866	58.240	54.621	52.373	108.756	100.199	92.518	86.137	81.117
0.540	71.416	63.084	57.564	54.012	51.788	107.164	98.857	91.401	85.201	80.306
0.560	70.444	62.256	56.848	53.365	51.164	105.487	97.439	90.216	84.203	79.436
0.580	69.415	61.380	56.089	52.677	50.500	103.720	95.940	88.958	83.139	78.504
0.600	68.328	60.453	55.284	51.946	49.792	101.859	94.356	87.624	82.004	77.504
0.620	67.181	59.469	54.863	51.163	49.040	100.892	93.531	86.927	81.409	76.977
0.630	67.178	59.471	54.430	51.167	49.037	99.899	92.683	86.208	80.793	76.431
0.640	66.578	58.929	53.983	50.761	48.690	98.879	91.810	85.468	80.157	75.865
0.650	65.961	58.431	53.524	50.341	48.230	97.833	90.913	84.704	79.499	75.278
0.660	65.325	57.888	53.049	49.907	47.806	96.758	89.990	83.917	78.819	74.669
0.670	64.671	57.229	52.561	49.458	47.368	95.654	89.040	83.105	78.115	74.037
0.680	63.997	56.752	52.056	48.995	46.914	94.520	88.062	82.267	77.387	73.382
0.690	63.303	56.158	51.536	48.516	46.444	93.355	87.056	81.403	76.634	72.702
0.700	62.588	55.545	50.999	48.021	45.958	92.158	86.020	80.510	75.853	71.995
0.710	61.851	54.913	50.444	47.509	45.453	90.927	84.952	79.588	75.045	71.261
0.720	61.090	54.261	49.871	46.978	44.931	89.662	83.852	78.636	74.207	70.496
0.730	60.306	53.588	49.278	46.429	44.388	88.360	82.718	77.651	73.338	69.704
0.730	59.495	52.892	48.665	45.859	43.825	87.019	81.548	76.632	72.436	68.878
0.740	58.659	52.173	48.030	45.268	43.240	85.639	80.341	75.578	71.499	68.017
0.750	57.794	51.429	47.373	44.654	42.631	84.217	79.093	74.486	70.526	67.121
0.760	56.899	50.659	46.691	44.017	41.998	82.751	77.805	73.354	69.514	66.185
0.770	55.972	49.861	45.983	43.353	41.338	81.238	76.472	72.179	68.460	65.209
0.780	55.012	49.033	45.248	42.662	40.650	79.677	75.092	70.960	67.363	64.189
0.790	54.016	48.174	44.483	41.942	39.932	78.063	73.663	69.693	66.218	63.122
0.800	52.982	47.281	43.687	41.190	39.181	76.394	72.181	68.374	65.022	62.005
0.810	51.907	46.352	42.856	40.403	38.396	74.667	70.642	67.000	63.772	60.833
0.820	50.788	45.383	41.989	39.579	37.572	72.876	69.042	65.567	62.463	59.603
0.820	49.621	44.373	41.081	38.715	36.707	71.017	67.376	64.070	61.090	58.310
0.840	48.402	43.316	40.130	37.807	35.798	69.084	65.639	62.503	59.648	56.948
0.850	47.126	42.208	39.130	36.849	34.839	67.072	63.825	60.859	58.130	55.511
0.860	45.788	41.045	38.077	35.838	33.827	64.973	61.926	59.132	56.529	53.992
0.870	44.381	39.821	36.965	34.767	32.756	62.777	59.933	57.312	54.834	52.381
0.880	42.897	38.527	35.787	33.629	31.618	60.476	57.835	55.389	53.037	50.668
0.890	41.326	37.156	34.533	32.415	30.407	58.058	55.621	53.350	51.124	48.842
0.900	39.657	35.697	33.193	31.114	29.113	55.498	53.274	51.179	49.079	46.887
0.905	38.781	34.930	32.487	30.427	28.431	54.165	52.046	50.038	48.002	45.856
0.910	37.875	34.135	31.754	29.713	27.725	52.790	50.776	48.857	46.883	44.765
0.915	36.935	33.310	30.991	28.970	26.991	51.369	49.462	47.634	45.711	43.572	42.313
0.920	35.959	32.453	31.096	28.195	26.228	49.901	48.100	46.357	44.511	41.513
0.925	34.944	31.560	29.366	27.386	25.433	48.379	46.691	45.030	43.249	41.304
0.930	33.885	30.628	28.497	26.538	24.604	46.799	45.213	43.646	41.930	40.039
0.935	32.779	29.652	27.584	25.647	23.737	45.155	43.677	42.198	40.547	38.714
0.940	31.618	28.627	26.623	24.712	22.829	43.440	42.070	40.679	39.095	37.322
0.945	30.397	27.547	25.608	23.724	21.875	41.644	40.383	39.080	37.563	35.855
0.950	29.107	26.402	24.529	22.677	20.870	39.757	38.606	37.390	35.942	34.302
0.955	27.737	25.187	23.378	21.562	19.807	37.765	36.724	35.595	34.219	32.652
0.960	26.274	23.884	22.143	20.370	18.677	35.651	34.719	33.678	32.377	30.889
0.965	24.700	22.472	20.806	19.087	17.469	33.391	32.569	31.615	30.393	28.991
0.970	22.989	20.947	19.344	17.694	16.169	30.953	30.242	29.375	28.239	26.931
0.975	21.107	19.256	17.732	16.167	14.753	28.292	27.691	26.913	25.870	24.668
0.980	18.998	17.354	15.956	14.486	13.187	25.337	24.847	24.160	23.220	22.139
0.985	16.569	15.170	13.922	12.627	11.413	21.970	21.589	21.000	20.180	19.238
0.990	13.642	12.470	11.304	10.223	9.313	17.961	17.689	17.209	16.535	15.762
0.995	9.720	8.883	8.095	7.419	6.592	12.717	12.554	12.213	11.731	11.192
1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

where $R_1^f(z)$ is given by (PP, 1977)

$$R_1^f(z) = \frac{2\sigma_B}{\pi\sigma_A} \ln\left(\frac{1+\sigma_A}{1-\sigma_A}\right). \qquad (42)$$

3. Discussion of the theoretical results

The theoretical expressions for the six normalized R indices valid for truncated data have been derived in (25), (29), (31), (34), (38) and (41). A study of these equations shows that we can, in general, write the R indices applicable to the truncated data in the general form as

$$[R]_t = A(y_t)\,[R + B(\sigma_A, y_t)], \qquad (43)$$

where R stands for any one of the normalized R indices, $A(y_t)$ is a function of y_t and $B(\sigma_A, y_t)$ is a function of σ_A and y_t. If $y_t \to 0$, $A(y_t) \to 1$ and $B(\sigma_A, y_t) \to 0$ so that $[R]_t \to R$ as required.

A study of (25), (29), (31), (34), (38) and (41) shows that these R indices depend on the parameters y_t (which is a characteristic of the data) and σ_A. σ_A is in turn a function of σ_1^2 (*i.e.* the fractional contribution to the local mean intensity from the known atoms), $\langle|\Delta\mathbf{r}|\rangle$ (*i.e.* the mean positional error in the atoms of the model) and $\sin\theta/\lambda$. Putting $\sigma_A = \sigma_1$ (*i.e.* $\langle|\Delta\mathbf{r}|\rangle = 0$) in these equations, we can obtain the results for the related case. Similarly, putting $\sigma_A = 0$ (*i.e.* $\langle|\Delta\mathbf{r}|\rangle$ large), we can obtain the results for the unrelated case. The local values of these R indices (in percent) are given in Tables 2–4 as functions of σ_A for different fixed values of y_t,

Table 3. *Values of* $[{}_BR_1(y)]_t$ *and* $[{}_BR_1(z)]_t$ *as functions of* σ_A *and* y_t *for the centrosymmetric case*

	$[{}_BR_1(y)]_t$					$[{}_BR_1(z)]_t$				
σ_A ↓	$y_t \to$ 0.00	0.15	0.30	0.45	0.60	$y_t \to$ 0.00	0.15	0.30	0.45	0.60
0.000	72.676	62.143	54.377	49.045	45.697	133.333	121.469	110.218	100.125	91.595
0.040	72.574	62.059	54.307	48.985	45.643	133.120	121.294	110.077	100.014	91.505
0.080	72.268	61.806	54.097	48.804	45.479	132.480	120.767	109.654	99.677	91.233
0.120	71.758	61.385	53.746	48.502	45.205	131.413	119.887	108.946	99.113	90.777
0.160	71.043	60.794	53.253	48.078	44.820	129.920	118.653	107.951	98.318	90.131
0.200	70.121	60.031	52.617	47.530	44.322	128.000	117.062	106.662	97.283	89.287
0.240	68.991	59.096	51.837	46.857	43.709	125.653	115.110	105.075	96.002	88.236
0.280	67.652	57.986	50.909	46.055	42.978	122.880	112.795	103.181	94.464	86.966
0.320	66.100	56.700	49.831	45.123	42.126	119.680	110.110	100.972	92.656	85.462
0.360	64.333	55.233	48.601	44.055	41.149	116.053	107.052	98.438	90.565	83.708
0.400	62.347	53.583	47.214	42.849	40.042	112.000	103.613	95.567	88.176	81.686
0.420	61.271	52.688	46.460	42.162	39.438	109.813	101.749	94.001	86.863	80.569
0.440	60.140	51.745	45.666	41.499	38.800	107.520	99.787	92.346	85.469	79.376
0.460	58.951	50.754	44.830	40.768	38.126	105.120	97.726	90.600	83.991	78.105
0.480	57.705	49.715	43.951	39.998	37.416	102.613	95.565	88.760	82.427	76.754
0.500	56.401	48.626	43.029	39.190	36.668	100.000	93.304	86.826	80.773	75.318
0.520	55.038	47.487	42.063	38.341	35.882	97.280	90.941	84.795	79.026	73.795
0.540	53.616	46.297	41.053	37.451	35.056	94.453	88.475	82.664	77.185	72.181
0.560	52.132	45.054	39.996	36.518	34.189	91.520	85.905	80.432	75.245	70.473
0.580	50.588	43.759	38.892	35.542	33.280	88.480	83.229	78.097	73.204	68.666
0.600	48.981	42.410	37.740	34.520	32.328	85.333	80.447	75.655	71.058	66.758
0.610	48.154	41.714	37.145	33.992	31.834	83.720	79.015	74.393	69.945	65.764
0.620	47.310	41.005	36.538	33.452	31.329	82.080	77.556	73.104	68.804	64.743
0.630	46.451	40.281	35.917	32.900	30.813	80.413	76.070	71.787	67.635	63.695
0.640	45.575	39.543	35.284	32.336	30.284	78.720	74.556	70.441	66.438	62.618
0.650	44.682	38.791	34.638	31.759	29.743	77.000	73.014	69.068	65.212	61.513
0.660	43.773	38.024	33.978	31.169	29.189	75.253	71.445	67.665	63.956	60.379
0.670	42.846	37.242	33.305	30.566	28.623	73.480	69.847	66.233	62.671	59.215
0.680	41.903	36.444	32.617	29.950	28.043	71.680	68.222	64.772	61.356	58.021
0.690	40.942	35.632	31.916	29.320	27.450	69.853	66.567	63.281	60.010	56.796
0.700	39.964	34.804	31.200	28.677	26.843	68.000	64.885	61.759	58.632	55.539
0.710	38.968	33.960	30.469	28.019	26.222	66.120	63.173	60.207	57.223	54.251
0.720	37.953	33.100	29.723	27.346	25.587	64.213	61.432	58.624	55.781	52.929
0.730	36.921	32.223	28.962	26.659	24.936	62.280	59.662	57.009	54.307	51.575
0.740	35.869	31.330	28.186	25.956	24.271	60.320	57.863	55.362	52.799	50.187
0.750	34.799	30.419	27.393	25.237	23.590	58.333	56.033	53.684	51.258	48.764
0.760	33.710	29.492	26.583	24.502	22.893	56.320	54.174	51.972	49.682	47.306
0.770	32.601	28.546	25.757	23.751	22.179	54.280	52.285	50.228	48.071	45.813
0.780	31.472	27.583	24.913	22.982	21.448	52.213	50.366	48.451	46.425	44.283
0.790	30.322	26.601	24.052	22.195	20.700	50.120	48.416	46.639	44.742	42.716
0.800	29.152	25.599	23.172	21.391	19.933	48.000	46.435	44.793	43.023	41.111
0.810	27.961	24.579	22.273	20.567	19.148	45.853	44.424	42.913	41.266	39.468
0.820	26.748	23.538	21.355	19.723	18.344	43.680	42.381	40.998	39.472	37.786
0.830	25.512	22.477	20.416	18.859	17.519	41.480	40.306	39.047	37.640	36.064
0.840	24.254	21.394	19.456	17.974	16.674	39.253	38.201	37.060	35.768	34.302
0.850	22.973	20.290	18.474	17.067	15.807	37.000	36.063	35.036	33.857	32.498
0.860	21.667	19.162	17.470	16.136	14.918	34.720	33.893	32.976	31.905	30.653
0.870	20.336	18.011	16.442	15.182	14.007	32.413	31.690	30.879	29.913	28.765
0.880	18.979	16.836	15.388	14.202	13.071	30.080	29.455	28.744	27.879	26.834
0.890	17.596	15.635	14.308	13.196	12.111	27.720	27.188	26.570	25.803	24.859
0.900	16.185	14.406	13.201	12.161	11.125	25.333	24.887	24.358	23.685	22.838
0.905	15.468	13.782	12.636	11.633	10.623	24.130	23.724	23.237	22.609	21.811
0.910	14.744	13.150	12.064	11.097	10.114	22.920	22.553	22.107	21.523	20.773
0.915	14.012	12.510	11.483	10.554	9.598	21.703	21.373	20.966	20.425	19.722
0.920	13.273	11.863	10.895	10.002	9.075	20.480	20.185	19.816	19.317	18.660
0.925	12.525	11.207	10.298	9.442	8.546	19.250	18.988	18.655	18.197	17.587
0.930	11.769	10.543	9.692	8.874	8.010	18.013	17.783	17.484	17.066	16.501
0.935	11.004	9.871	9.077	8.296	7.467	16.770	16.569	16.304	15.923	15.404
0.940	10.230	9.189	8.452	7.710	6.918	15.520	15.347	15.113	14.769	14.294
0.945	9.447	8.498	7.817	7.114	6.362	14.263	14.116	13.911	13.604	13.172
0.950	8.654	7.797	7.171	6.509	5.800	13.000	12.877	12.700	12.427	12.038
0.955	7.851	7.085	6.514	5.894	5.232	11.730	11.629	11.478	11.238	10.892
0.960	7.038	6.362	5.845	5.269	4.658	10.453	10.372	10.245	10.038	9.733
0.965	6.213	5.627	5.163	4.634	4.080	9.170	9.106	9.002	8.826	8.561
0.970	5.375	4.879	4.468	3.990	3.499	7.880	7.832	7.748	7.602	7.377
0.975	4.525	4.116	3.758	3.337	2.915	6.583	6.549	6.484	6.365	6.180
0.980	3.660	3.339	3.033	2.676	2.330	5.280	5.257	5.209	5.117	4.970
0.985	2.779	2.540	2.293	2.009	1.745	3.970	3.956	3.923	3.856	3.748
0.990	1.880	1.721	1.537	1.339	1.161	2.653	2.646	2.626	2.583	2.512
0.995	0.957	0.875	0.770	0.669	0.580	1.330	1.328	1.319	1.298	1.262
1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

since these are needed for evaluating the overall values of the R indices for a given situation (see later).

The variations of the R indices as a function of y_t for different fixed values of σ_1^2 have been obtained with the results in Tables 2–4 and the results obtained are shown in Figs. 1(*a*)–1(*f*). These figures have been obtained for the typical case where $\langle|\Delta\mathbf{r}|\rangle = 0{\cdot}2$ Å and $\sin\theta/\lambda = 0{\cdot}4$ Å^{-1}. From a study of these figures, we obtain the following results. (i) As y_t increases the value of R decreases. However, for $y_t > 0{\cdot}3$ this decrease is less marked. (ii) The decrease in R with y_t is more marked when σ_1^2 is small than when it is close to unity. Since for the data of actual crystals y_t is expected to be in the neighbourhood of 0·2 (Ponnuswamy & Parthasarathy, 1977), it would be useful to take care of data truncation for the calculation of the theoretical overall values of R indices. In view of (ii) this is particularly true for incomplete models.

We shall summarize here the general procedure that may be followed for computing the theoretical overall values of R for a given model. During the structure completion stage, since the atoms added to the model are subject to positional errors of the order of 0·2 Å on average, one may set $\langle|\Delta\mathbf{r}|\rangle \simeq 0{\cdot}2$ Å. The evaluation of $[\bar{R}]_t$ involves the following steps. (i) From an analysis of the F_o data, determine the value of y_t appropriate to the data. (ii) Determine σ_1^2 for the given model. For a structure with similar atoms this may be taken to be

Table 4. *Values of* $[R_1^f(y)]_t$ *and* $[R_1^f(z)]_t$ *as functions of* σ_A *and* y_t *for the centrosymmetric case*

	$[R_1^f(y)]_t$					$[R_1^f(z)]_t$				
σ_A ↓ / y_t →	0·00	0·15	0·30	0·45	0·60	0·00	0·15	0·30	0·45	0·60
0·000	88·254	80·165	76·974	76·335	77·357	127·324	120·338	116·383	114·867	115·321
0·040	88·223	80·133	76·942	76·301	77·319	127·290	120·301	116·345	114·827	115·277
0·080	88·129	80·036	76·844	76·199	77·205	127·188	120·191	116·232	114·709	115·147
0·120	87·971	79·873	76·681	76·028	77·013	127·016	120·006	116·041	114·509	114·927
0·160	87·748	79·643	76·451	75·786	76·742	126·773	119·745	115·771	114·227	114·615
0·200	87·457	79·344	76·150	75·471	76·388	126·456	119·403	115·419	113·858	114·209
0·240	87·097	78·973	75·778	75·080	75·948	126·061	118·979	114·981	113·399	113·701
0·280	86·662	78·525	75·328	74·607	75·417	125·584	118·466	114·452	112·844	113·087
0·320	86·149	77·997	74·798	74·049	74·788	125·019	117·858	113·826	112·186	112·358
0·360	85·552	77·383	74·181	73·398	74·053	124·359	117·148	113·093	111·416	111·502
0·400	84·862	76·675	73·470	72·646	73·203	123·593	116·325	112·245	110·523	110·508
0·420	84·481	76·283	73·076	72·230	72·731	123·168	115·868	111·774	110·026	109·953
0·440	84·073	75·865	72·655	71·784	72·225	122·712	115·378	111·269	109·492	109·358
0·460	83·637	75·418	72·206	71·307	71·684	122·223	114·854	110·728	108·921	108·719
0·480	83·172	74·941	71·726	70·797	71·104	121·700	114·292	110·148	108·308	108·032
0·500	82·675	74·432	71·214	70·253	70·485	121·139	113·691	109·528	107·651	107·296
0·520	82·145	73·889	70·667	69·671	69·822	120·539	113·047	108·864	106·946	106·505
0·540	81·580	73·311	70·085	69·049	69·112	119·896	112·358	108·153	106·191	105·655
0·560	80·976	72·693	69·463	68·384	68·353	119·206	111·619	107·391	105·380	104·742
0·580	80·331	72·034	68·798	67·673	67·539	118·467	110·827	106·573	104·509	103·759
0·600	79·641	71·330	68·088	66·911	66·666	117·672	109·977	105·696	103·573	102·700
0·610	79·279	70·960	67·715	66·510	66·206	117·253	109·528	105·233	103·078	102·140
0·620	78·903	70·577	67·328	66·094	65·729	116·818	109·063	104·752	102·563	101·558
0·630	78·515	70·181	66·929	65·664	65·234	116·366	108·580	104·254	102·029	100·953
0·640	78·112	69·771	66·514	65·217	64·721	115·897	108·079	103·736	101·474	100·323
0·650	77·696	69·347	66·085	64·754	64·188	115·410	107·558	103·198	100·897	99·668
0·660	77·263	68·907	65·640	64·273	63·635	114·903	107·017	102·639	100·296	98·986
0·670	76·815	68·451	65·179	63·774	63·061	114·376	106·454	102·058	99·671	98·275
0·680	76·350	67·978	64·700	63·255	62·463	113·827	105·869	101·453	99·019	97·533
0·690	75·867	67·487	64·203	62·716	61·842	113·255	105·259	100·822	98·339	96·760
0·700	75·364	66·977	63·686	62·154	61·195	112·659	104·624	100·165	97·629	95·952
0·710	74·842	66·448	63·149	61·570	60·521	112·037	103·961	99·480	96·888	95·107
0·720	74·299	65·897	62·590	60·960	59·819	111·388	103·269	98·764	96·113	94·223
0·730	73·733	65·323	62·008	60·324	59·086	110·708	102·546	98·015	95·301	93·298
0·740	73·143	64·726	61·400	59·660	58·320	109·997	101·790	97·232	94·450	92·327
0·750	72·527	64·102	60·766	58·966	57·520	109·252	100·997	96·411	93·557	91·309
0·760	71·883	63·452	60·103	58·239	56·682	108·470	100·167	95·549	92·619	90·239
0·770	71·209	62·771	59·410	57·477	55·804	107·649	99·294	94·644	91·631	89·113
0·780	70·504	62·059	58·683	56·677	54·884	106·784	98·377	93·692	90·590	87·927
0·790	69·763	61·313	57·920	55·835	53·917	105·873	97·410	92·687	89·490	86·675
0·800	68·985	60·529	57·118	54·949	52·900	104·910	96·390	91·626	88·327	85·351
0·810	68·165	59·704	56·276	54·014	51·828	103·891	95·310	90·503	87·093	83·950
0·820	67·300	58·835	55·390	53·025	50·697	102·809	94·167	89·312	85·782	82·463
0·830	66·386	57·917	54·456	51·977	49·502	101·660	92·951	88·044	84·385	80·882
0·840	65·416	56·945	53·434	50·863	48·237	100·433	91·656	86·691	82·892	79·198
0·850	64·385	55·913	52·368	49·676	46·894	99·121	90·272	85·244	81·293	77·399
0·860	63·286	54·814	51·229	48·408	45·465	97·712	88·788	83·688	79·572	75·472
0·870	62·108	53·638	50·008	47·047	43·942	96·192	87·189	82·010	77·714	73·403
0·880	60·842	52·376	48·694	45·582	42·314	94·546	85·458	80·190	75·699	71·172
0·890	59·474	51·015	47·271	43·997	40·569	92·752	83·576	78·206	73·503	68·760
0·900	57·987	49·538	45·721	42·274	38·693	90·786	81·516	76·029	71·096	66·139
0·905	57·192	48·749	44·892	41·354	37·700	89·727	80·408	74·856	69·801	64·742
0·910	56·358	47·923	44·021	40·391	36·669	88·612	79·242	73·620	68·439	63·280
0·915	55·483	47·056	43·105	39·380	35·595	87·435	78·013	72·313	67·003	61·749
0·920	54·561	46·145	42·140	38·318	34·477	86·188	76·712	70·929	65·485	60·143
0·925	53·587	45·182	41·119	37·199	33·311	84·864	75·331	69·459	63·877	58·455
0·930	52·554	44·164	40·038	36·018	32·094	83·453	73·861	67·890	62·170	56·678
0·935	51·457	43·081	38·883	34·769	30·822	81·943	72·290	66·211	60·351	54·804
0·940	50·285	41·924	37·651	33·444	29·491	80·319	70·603	64·405	58·408	52·823
0·945	49·027	40·690	36·327	32·035	28·096	78·566	68·783	62·455	56·325	50·722
0·950	47·670	39·356	34·900	30·531	26·633	76·659	66·806	60·335	54·082	48·488
0·955	46·196	37·909	33·349	28·922	25·094	74·571	64·644	58·016	51·655	46·104
0·960	44·581	36·324	31·654	27·193	23·473	72·264	62·258	55·459	49·015	43·548
0·965	42·794	34·572	29·784	25·326	21·760	69·686	59·596	52·613	46·125	40·792
0·970	40·790	32·608	27·702	23·301	19·944	66·766	56·584	49·408	42·935	37·801
0·975	38·504	30·368	25·352	21·088	18·003	63·395	53·111	45·745	39·374	34·520
0·980	35·831	27·749	22·661	18·649	15·909	59·402	49·002	41·479	35·342	30·871
0·985	32·591	24·573	19·513	15·919	13·603	54·483	43·949	36·376	30·670	26·720
0·990	28·412	20·486	15·714	12·766	10·960	48·018	37·335	30·004	25·041	21·813
0·995	22·278	14·602	10·819	8·801	7·654	38·271	27·551	21·325	17·627	15·523
1·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000	0·000

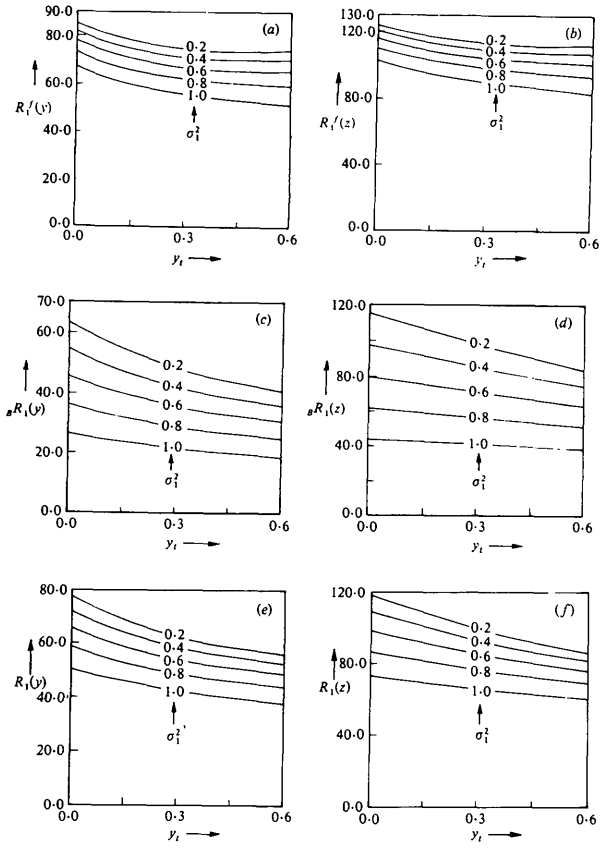

Fig. 1. Variation of the local values of normalized R indices as a function of y_t for different fixed values of σ_1^2. For the definition of $R_1(y)$, $R_1(z)$, *etc.*, see column 6 of Table 1.

P/N. (iii) Divide the range $0 \le s \le S_{max}$ into a number of narrow subintervals. Determine from the data the number (n_s) of observed reflections in each of these sub-intervals. (iv) From the mean value of $\sin\theta/\lambda$ corresponding to each sub-interval determine the values of f. (v) Calculate σ_A (by taking $\langle|\Delta\mathbf{r}|\rangle = 0{\cdot}2$ Å) corresponding to each of these sub-intervals. (vi) Make use of the results in Tables 2–4 and determine the values of $[R]_t$ for these sub-intervals by bilinear interpolation. (vii) Make use of the results thus obtained in the appropriate expressions for $[\bar{R}]_t$ and compute the overall values $[\bar{R}]_t$. The values thus obtained represent the theoretical overall values of the normalized R indices corresponding to a model for which $\langle|\Delta\mathbf{r}|\rangle = 0{\cdot}2$ Å and for data in which $y_N \ge y_t$ and $0 \le s \le S_{max}$.

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Theoretical Evaluation of the Overall Values of Discrepancy Indices for Truncated Data. II. Normalized R indices for a Non-centrosymmetric Crystal with Similar Atoms

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Abstract

Theoretical expressions and numerical tables for the local values of six types of normalized R indices are obtained for an imperfectly related incomplete model of a non-centrosymmetric crystal with truncated data. Under similar conditions, the curve of the local value of an R index *versus* the truncation limit y_t is relatively more flat for the non-centrosymmetric case than for the centrosymmetric case particularly in the region where y_t is small.

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