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Overall values of conventional discrepancy indices for related and unrelated models of a non-centrosymmetric crystal with a centrosymmetric group*

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Abstract. Theoretical expressions for the overall values of the conventional discrepancy indices $R(F)$ and $R(I)$ are derived for a non-centrosymmetric crystal with a centrosymmetric group by taking the centrosymmetric group and a part of the other atoms in the unit cell as the trial structure. These results are used to obtain tables of values of these indices in terms of the parameter σ_{1c}^1 and σ_1^1 which define the fractional contribution to the local mean intensity from the centrosymmetric group and all the known atoms respectively.

Keywords. Conventional discrepancy indices; noncentrosymmetric crystal; centrosymmetric group; local mean intensity.

1. Introduction

Theoretical overall values of the conventional R-indices $R(F)$ and $R(I)$ have been obtained for a crystal with similar atoms in the unit cell for the following two situations: (i) a non-centrosymmetric (NC, hereafter) crystal obeying the acentric Wilson distribution and (ii) for a centrosymmetric (C, hereafter) crystal obeying the centric Wilson distribution (Parthasarathy and Ponnuswamy 1979). Theoretical overall values of these indices have not so far been obtained for a NC crystal with similar atoms containing a C group (*e.g.*, a benzene-like ring) as a part of the structure. In this paper we shall therefore derive the theoretical expressions for the overall values of $R(F)$ and $R(I)$ [denoted by $\overline{R}(F)$ and $\overline{R}(I)$ respectively] for such a situation by taking the model to consist of the centrosymmetric group and a *part* of the other light atoms in the unit cell. Results are derived for both the related case (*i.e.*, the model is perfectly correct) and the unrelated case (*i.e.*, the model is completely wrong). We shall assume all the atoms in the unit cell to be of similar scattering power.

2. Derivation of the theoretical expressions for the overall values of R(F) and R(I)

2.1 *Notation and preliminary results*

Consider an *NC* crystal (space group $P1$) containing N similar atoms in the unit cell.

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Let there be a *single C* group consisting of P_c atoms in the unit cell. At a given stage of structure determination, let the trial structure consist of the *C* group of atoms besides a group of P_n atoms in an *NC* configuration. Thus the known group with *P* atoms will be made up of an *NC* group of P_n atoms and a *C* group of P_c atoms. That is, $P = P_n + P_c$. Let *Q* be the number of atoms in the unit cell yet to be located. Then $N = P + Q$. The structure factor of a reflection $\mathbf{H}(= hkl)$ can be written in terms of the contributions from the individual groups of atoms as

$$F_N = F_P + F_Q = F_{Pc} + F_{Pn} + F_Q. \tag{1}$$

Let F_P^c denote the calculated structure factor for the reflection **H** due to the contributions from the *P* atoms of the model. The contributions to the local mean intensity from the various groups of atoms can be written as

$$\langle |F_\alpha|^2 \rangle = \sum_{j=1}^{\alpha} f_{\alpha j}^2 = \sigma_{\alpha j}^2, \quad \langle |F_P^c|^2 \rangle = \sum_{j=1}^{P} f_{Pj}^2 = \sigma_P^2, \tag{2}$$

where α stands for N, P, Q, P_c or P_n. Let the fractional contributions to the local mean intensity from the P, P_c, P_n and Q groups be denoted by σ_1^2, σ_{1c}^2, σ_{1n}^2 and σ_2^2 respectively. From (2) it follows that

$$\sigma_1^2 = \langle |F_P|^2 \rangle / \langle |F_n|^2 \rangle = \sigma_P^2 / \sigma_N^2,$$

$$\sigma_{1c}^2 = \langle |F_{Pc}|^2 \rangle / \langle |F_N|^2 \rangle = \sigma_{Pc}^2 / \sigma_N^2,$$

$$\sigma_{1n}^2 = \langle |F_{Pn}|^2 \rangle / \langle |F_N|^2 \rangle = \sigma_{Pn}^2 / \sigma_N^2,$$

$$\sigma_2^2 = \langle |F_Q|^2 \rangle / \langle |F_N|^2 \rangle = \sigma_Q^2 / \sigma_N^2. \tag{3}$$

For the equal-atom case (3) can be shown to reduce to

$$\sigma_1^2 = P/N, \quad \sigma_{1c}^2 = P_c/N, \quad \sigma_{1n}^2 = P_n/N, \quad \sigma_2^2 = Q/N, \tag{4}$$

which are independent of $\sin\theta/\lambda$ (S, hereafter). From (4) it follows that

$$\sigma_1^2 + \sigma_2^2 = 1, \qquad \sigma_{1c}^2 + \sigma_{1n}^2 = \sigma_1^2. \tag{5}$$

The normalized structure amplitudes y_N and y_P^c are defined in the usual way, namely,

$$y_N = |F_N| / \langle |F_N|^2 \rangle^{1/2}, \quad y_P^c = |F_{Pc}| / \langle |F_{Pc}|^2 \rangle^{1/2}. \tag{6}$$

It may be noted that for the related case $|F_P^c| = |F_P|$ so that $y_P^c = y_P$ while for the unrelated case y_P and y_P^c are independent random variables.

2.2 *Expression for* $\bar{R}(F)$

Following the arguments of Parthasarathy and Ponnuswamy (1979), the overall value of $R(F)$ for an incomplete model (of the related or unrelated type) can be written as

$$\bar{R}(F) = \frac{\sum_{hkl} \left| |F_N| - |F_P^c| \right|}{\sum_{hkl} |F_N|} = \frac{\sum_j \sigma_{Nj} n_j \langle |y_N - \sigma_1 y_P^c| \rangle_j}{\sum_j \sigma_{Nj} n_j \langle y_N \rangle_j}. \qquad (7a, b)$$

The derivation of (7b) from (7a) involves the partitioning of the reciprocal space into thin shells. The subscripts j to a quantity denotes that the quantity pertain to the jth shell. n_j denotes the number of independent reflections in the jth shell.

It will be shown later that for crystals with similar atoms and for related and unrelated models the quantities $\langle |y_N - \sigma_1 y_P^c| \rangle$ and $\langle y_N \rangle$ will be practically independent of S. These quantities can therefore be factored out of the summation symbols in (7b) so that

$$\bar{R}(F) = \frac{\langle |y_N - \sigma_1 y_P^c| \rangle}{\langle y_N \rangle}. \qquad (8)$$

In order to obtain $\bar{R}(F)$ for the related or unrelated case we must therefore first evaluate the quantities $\langle |y_N - \sigma_1 y_P^c| \rangle$ and $\langle y_N \rangle$ and we shall presently consider this aspect.

2.2a *Theoretical expressions for* $\langle |y_N - \sigma_1 y_P^c| \rangle$ *and* $\langle y_N \rangle$: If $P(y_N, y_P^c)$ is the joint pdf of y_N and y_P^c then $\langle |y_N - \sigma_1 y_P^c| \rangle$ will be given by

$$\langle |y_N - \sigma_1 y_P^c| \rangle = \int_0^\infty \int_0^\infty |y_N - \sigma_1 y_P^c| \, P(y_N, y_P^c) \, dy_N \, dy_P^c. \qquad (9)$$

Since $P(y_N, y_P^c)$ for the related and unrelated cases turn out to be complicated functions (see later) the integrals in (9) cannot be evaluated in a closed form. To facilitate evaluation by numerical methods, it is found to be convenient to change the variables of integrations from (y_N, y_P^c) to (u, v) by using the transformation

$$y_N = u/(1-u), \quad y_P^c = v/(1-v). \qquad (10)$$

Thus we can rewrite (9) as

$$\langle |y_N - \sigma_1 y_P^c| \rangle = \int_0^1 \int_0^1 \left| \left(\frac{u}{1-u}\right) - \sigma_1 \left(\frac{v}{1-v}\right) \right| P\left(\frac{u}{1-u}, \frac{v}{1-v}\right) \frac{du\, dv}{(1-u)^2 (1-v)^2}. \qquad (11)$$

It is obvious that $\langle y_N \rangle$ will depend only on the structure but not on the model. Hence $\langle y_N \rangle$ will be given by the same expression for both the related and unrelated cases. From (3.86) of Srinivasan and Parthasarathy (1976) we can show that

$$\langle y_N \rangle = \left(\frac{1+\sigma_{1c}^2}{\pi}\right)^{1/2} E\left(\frac{2\sigma_{1c}^2}{1+\sigma_{1c}^2}\right)^{1/2}. \tag{12}$$

2.3 *General expression for the overall value of R(I)*

Starting from the definition of $\bar{R}(I)$, namely,

$$\bar{R}(I) = \frac{\sum\limits_{hkl} |I_N - I_P^c|}{\sum\limits_{hkl} I_N} = \frac{\sum\limits_{hkl} ||F_N|^2 - |F_P^c|^2|}{\sum\limits_{hkl} |F_N|^2}, \tag{13}$$

and following the arguments used for obtaining (7b) from (7a) we can show that

$$\bar{R}(I) = \frac{\sum\limits_j \sigma_{Nj}^2 n_j \langle |y_N^2 - \sigma_1^2 y_P^{c2}| \rangle_j}{\sum\limits_j \sigma_{Nj}^2 n_j}, \tag{14}$$

where we have used the known result that $\langle y_N^2 \rangle = 1$. Since $\langle |y_N^2 - \sigma_1^2 y_P^{c2}| \rangle$ is practically independent of S for the related and unrelated models of crystals containing similar atoms, this quantity can be factored out of the summation symbol in the numerator of (14). We thus obtain

$$\bar{R}(I) = \langle |y_N^2 - \sigma_1^2 y_P^{c2}| \rangle. \tag{15}$$

Making use of the $P(y_N, y_P^c)$ we can write (15) as

$$\bar{R}(I) = \int_0^\infty \int_0^\infty |y_N^2 - \sigma_1^2 y_P^{c2}| \, P(y_N, y_P^c) \, dy_N \, dy_P^c$$

$$= \int_0^1 \int_0^1 \left| \left(\frac{u}{1-u}\right)^2 - \sigma_1^2 \left(\frac{v}{1-v}\right)^2 \right| P\left(\frac{u}{1-u}, \frac{v}{1-v}\right) \frac{du\, dv}{(1-u)^2 (1-v)^2}, \tag{16a, b}$$

where we have used the transformation in (10) for obtaining (16b) from (16a).

It is useful to note the following points with regard to the evaluation of $\bar{R}(F)$ and $\bar{R}(I)$ from the above results: Since no results arising from any particular feature of either the related or the unrelated case were invoked in the above theoretical

considerations, all these results are valid for both the related and unrelated cases. However since $y_P^c = y_P$ for the related case we shall use y_P instead of y_P^c in these expressions when they are applied to the related case.

It is seen from (11) and (16b) that for evaluation of $\overline{R}(F)$ and $\overline{R}(I)$ we must first derive the theoretical expression of $P(y_N, y_P)$ for the related case and of $P(y_N, y_P^c)$ for the unrelated case. We shall consider this aspect presently.

2.4 *Derivation of $P(y_N, y_P)$ for the related case*

$P(y_N, y_P)$ is related to the conditional pdf of y_N for a given y_P and the pdf of y_P by

$$P(y_N, y_P) = P(y_N; y_P)\, P(y_P). \tag{17}$$

Assuming the Q-group to consist of a sufficiently large number of atoms so as to satisfy the requirements of the acentric Wilson distribution, $P(y_N, y_P^c)$ (whatever be the nature of the P-group) has been shown to be (see (3·24) of Srinivasan and Parthasarathy 1976)

$$P(y_N; y_P) = \frac{2y_N}{\sigma_2^2} \exp\left[-\frac{(y_N^2 + \sigma_1^2 y_P^2)}{\sigma_2^2}\right] I_0\left[\frac{2\sigma_1 y_N y_P}{\sigma_2^2}\right]. \tag{18}$$

It is obvious that $P(y_P)$ required for the present case is to be obtained from the expression for $P(y)$ in equation (8) of Parthasarathy (1966) by replacing the set $(y, \sigma_1^2 = \sigma_P^2/\sigma_N^2, \sigma_2^2 = \sigma_Q^2/\sigma_N^2)$ by the set $(y_P, \sigma_{Pc}^2/\sigma_P^2, \sigma_{Pn}^2/\sigma_P^2)$. Making use of (3) we can show that

$$\sigma_{Pc}^2/\sigma_P^2 = \sigma_{1c}^2/\sigma_1^2,\ \sigma_{Pn}^2/\sigma_P^2 = \sigma_{1n}^2/\sigma_1^2$$

We hence obtain $P(y_P)$ to be

$$P(y_P) = \frac{2\sigma_1^2 y_P}{[\sigma_{1n}^2(\sigma_{1n}^2 + \sigma_{1c}^2)]^{1/2}} \exp\left[-\frac{\sigma_1^4 y_P^2}{\sigma_{1n}^2(\sigma_1^2 + \sigma_{1c}^2)}\right] I_0\left[\frac{\sigma_1^2 \sigma_{1c}^2 y_P^2}{\sigma_{1n}^2(\sigma_1^2 + \sigma_{1c}^2)}\right]. \tag{19}$$

Substituting (18) and (19) in (17) we obtain

$$P(y_N, y_P) = \frac{4\sigma_1^2 y_N y_P}{\sigma_2^2[\sigma_{1n}^2(\sigma_1^2+\sigma_{1c}^2)]^{1/2}} \exp\left[-\frac{y_N^2}{\sigma_2^2} - \frac{\sigma_1^2\{\sigma_{1n}^2(\sigma_1^2+\sigma_{1c}^2)+\sigma_1^2\sigma_2^2\}}{\sigma_2^2\sigma_{1n}^2(\sigma_1^2+\sigma_{1c}^2)} y_p^2\right] \times$$

$$I_0\left[\frac{2\sigma_1 y_N y_P}{\sigma_2^2}\right] I_0\left[\frac{\sigma_1 \sigma_{1c} y_P^2}{\sigma_{1n}^2(\sigma_1^2+\sigma_{1c}^2)}\right]. \tag{20}$$

It is seen that $P(y_N, y_P)$ in (20) depends on the parameters σ_{1c}^2 and σ_1^2 (Note that $\sigma_{1n}^2 = \sigma_1^2 - \sigma_{1c}^2$). From (5) it is clear that for a structure with similar atoms σ_{1c}^2 and σ_1^2 will be practically independent of S. Thus for any particular trial structure of a

crystal structure (with similar atoms), $P(y_N, y_P)$ and (consequently) the quantities $\langle |y_N - \sigma_1 y_P| \rangle$, $\langle |y_N^2 - \sigma_1^2 y_P^2| \rangle$ and $\langle y_N \rangle$ will be practically independent of the value of S. It may be noted that this fact was used for deriving (8) from (7b) and (15) from (14). Substituting (20) in (11) and (16b) the theoretical expressions for $\langle |y_N^n - \sigma_1 y_P^n| \rangle$, $n = 1, 2$, can be obtained. These two quantities for a given related model (i.e., for given $\sigma^2{}_c$ and σ_1^2) are to be obtained by carrying out the integrations in (11) and (16b) numerically.

2.5 *Derivation of $P(y_N, y_P^c)$ for the unrelated case*

For the unrelated case y_N and y_P^c are independent random variables so that

$$P(y_N, y_P^c) = P(y_N)\, P(y_P^c). \tag{21}$$

It is obvious that $P(y_N)$ required in (21) is to be obtained from the expression for $P(y)$ in equation (8) of Parthasarathy (1966) by replacing the set $(y, \sigma_1^2, \sigma_2^2)$ by the set $(y_N, \sigma_1^2, \sigma_{1n}^2+\sigma_2^2=1-\sigma_{1c}^2)$ which is the equivalent of the set $[y_N, \sigma_{Pc}^2/\sigma_N^2, \sigma_{Pn}^2+\sigma_Q^2)/\sigma_N^2]$. We thus obtain $P(y_N)$ to be

$$P(y_N) = \frac{2\, y_N}{(1-\sigma_{1c}^4)^{1/2}} \exp\left[-\frac{y_N^2}{(1-\sigma_{1c}^4)}\right] I_0\left[\frac{\sigma_{1c}^2\, y_N^2}{1-\sigma_{1c}^4}\right]. \tag{22}$$

It is obvious that $P(y_P^c)$ for the unrelated case will also be given by (19) (Note that y_P in (19) is now to be replaced by y_P^c). Making use of (19) and (22) in (21) we obtain

$$P(y_N, y_P^c) = \frac{4\, \sigma_1^2\, y_N\, y_P^c}{[\sigma_{1n}^2\,(\sigma_1^2+\sigma_{1c}^2)\,(1-\sigma_{1c}^4)]^{1/2}} \exp\left[-\frac{y_N^2}{1-\sigma_{1c}^4} - \frac{\sigma_1^4\, y_P^{c^2}}{\sigma_{1n}^2\,(\sigma_1^2+\sigma_{1c}^2)}\right] \times$$

$$I_0\left[\frac{\sigma_{1c}^2\, y_N^2}{1-\sigma_{1c}^4}\right] I_0\left[\frac{\sigma_1^2\, \sigma_{1c}^2\, y_P^{c^2}}{\sigma_{1n}^2\,(\sigma_1^2+\sigma_{1c}^2)}\right]. \tag{23}$$

Substituting (23) in (11) and (16b) and carrying out the resulting integrations numerically, the quantities $\langle |y_N^n - \sigma_1^n\, y_P^{cn}| \rangle$, $n = 1, 2$ for any unrelated model can be evaluated. Since σ_{1c}^2 and σ_1^2 for a structure with similar atoms are independent of S, it follows from (23) that $\langle |y_N^n - \sigma_1^n\, y_P^{cn}| \rangle$, $n = 1, 2$ for the unrelated case will be independent of the value of S.

2.6 *Derivation of $P(y_N, y_P)$ and $P(y_N, y_P^c)$ corresponding to the limiting situation $\sigma_{1n}^2 = 0$*

It is more easy to derive $P(y_N, y_P)$ and $P(y_N, y_P^c)$ required for the limiting situation $\sigma_{1n}^2 = 0$ (i.e., for the case where the P-group is completely centrosymmetric) directly

than by a limiting process from the distributions (20) and (23). In this connection it is useful to note the following: (i) If $\sigma_{1n}^2 = 0$ then $\sigma_{1c} = \sigma_1$ and (ii) $P(y_N, y_P^c)$ and $P(y_N)$ obtained in (18) and (22) are also valid for the present limiting situation.

If the P-group is assumed to consist only of a C group of atoms then y_P will follow the centric Wilson distribution, namely,

$$P(y_P) = (2/\pi)^{1/2} \exp(-y_P^2/2). \tag{24}$$

Substituting (18) and (24) in (17) we obtain the required $P(y_N, y_P)$ to be

$$P(y_N, y_P) = 2(2/\pi)^{1/2} \frac{y_N}{\sigma_2^2} \exp\left[-\frac{y_N^2}{2} - \frac{(1+\sigma_1^2) y_P^{c^2}}{2\sigma_2^2}\right] I_0\left[\frac{2\sigma_1 y_N y_P}{\sigma_2^2}\right]. \tag{25}$$

$P(y_P^c)$ for the present situation will evidently be the same function as that in (24). Substituting (22) and (24) (with y_P replaced by y_P^c) in (21) we obtain the required $P(y_N, y_P^c)$ to be

$$P(y_N, y_P^c) = 2\left(\frac{2}{\pi(1-\sigma_1^4)}\right)^{1/2} \exp\left[-\frac{y_N^2}{1-\sigma_1^4} - \frac{y_P^{c^2}}{2}\right] I_0\left[\frac{\sigma_1^2 y_N^2}{1-\sigma_1^4}\right]. \tag{26}$$

It may be noted that the expression for $\langle y_N \rangle$ in (12) is valid for the present limiting situation as well.

3. Discussion of the theoretical results

The theoretical evaluation of $\bar{R}(F)$ and $\bar{R}(I)$ requires that of $\langle | y_N^n - \sigma_1^n y_P^{c^n} | \rangle$, $n=1, 2$ and $\langle y_N \rangle$ [see (8), (12) and (15)]. Of these $\langle y_N \rangle$ is a function of σ_{1c}^2 alone [see (12)]. However $\langle | y_N^n - \sigma_1^n y_P^{c^n} | \rangle$, $n=1, 2$ depend on both σ_{1c}^2 and σ_1^2 since $P(y_N, y_P^c)$ contains these as parameters. For a given model of a crystal with similar atoms, σ_{1c}^2 and σ_1^2 are fixed quantities and hence are independent of S. The overall values of $R(F)$ and $R(I)$ for a given model can therefore be readily computed from (8) and (15) by substituting the values of $\langle | y_N^n - \sigma_1^n y_P^{c^n} | \rangle$, $n=1, 2$ and $\langle y_N \rangle$ calculated by using the values of σ_{1c}^2 and σ_1^2 appropriate to the model. Since the integrals involved in the evaluation of $\langle | y_N^n - \sigma_1^n y_P^{c^n} | \rangle$, $n=1, 2$ are complicated they were evaluated numerically for different fixed values of σ_{1c}^2 and σ_1^2. The values of $\bar{R}(F)$ thus obtained as a function of σ_{1c}^2 and σ_1^2 are given in table 1 and those for $\bar{R}(I)$ in table 2. The theoretical values of $\bar{R}(F)$ and $\bar{R}(I)$ for the related and unrelated cases corresponding to a given σ_{1c}^2 and σ_1^2 (determined by the model) can be obtained from these tables by interpolation.

Table 1. Overall value $\bar{R}$ (F) (in %) as a function of σ_{1c}^2 and σ_1^2 for the related and unrelated cases: A non-centrosymmetric crystal with a centrosymmetric group in the unit cell.

σ_1^2 \ σ_{1c}^2		0.00	0.05	0·10	0·15	0·20	0·30	0·40	0·50	0.60	0·70	0·80	0.90
0·00	R	100·00											
	UR	100·00											
0·05	R	78·64	80·97										
	UR	78·72	81·13										
0·10	R	70·95	71·49	74·19									
	UR	71·32	71·95	74·92									
0·15	R	65·58	65·84	66·74	69·37								
	UR	66·50	66·85	68·01	71·07								
0·20	R	61·33	61·48	61·96	62·95	65·46							
	UR	63·05	63·28	64·01	65·41	68·47							
0·25	R	57·83	57·92	58·22	58·77	59·76							
	UR	60·58	60·75	61·26	62·20	63·73							
0·30	R	54·65	54·71	54·90	55·25	55·83	59·02						
	UR	58·65	58·78	59·17	59·87	60·93	65·56						
0·35	R	51·90	51·94	52·07	52·30	52·66	54·14						
	UR	57·36	57·46	57·78	58·32	59·13	61·95						
0·40	R	49·24	49·27	49·36	49·52	49·77	50·66	53·50					
	UR	56·38	56·46	56·72	57·16	57·82	59·94	64·61					
0·45	R	46·59	46·61	46·67	46·79	46·96	47·56	48·90					
	UR	55·59	55·66	55·88	56·26	56·81	58·52	61·55					
0·50	R	44·22	44·24	44·29	44·37	44·50	44·91	45·73	48·22				
	UR	55·26	55·33	55·52	55·84	56.31	57·75	60·12	64·83				
0·55	R	41·75	41·76	41·80	41·87	41.96	42.26	42.80	43.94				
	UR	55.06	55.11	55.28	55.57	55.98	57.23	59.19	62.39				

0·60	R	39·24	39·25	39·28	39·33	39·40	39·61	39·99	40·67	42·83								
	UR	55·02	55·07	55·23	55·49	55·85	56·96	58·66	61·23	66·04								
0·65	R	36·48	36·48	36·51	36·54	36·60	36·77	37·04	37·49	38·44								
	UR	55·03	55·08	55·22	55·45	55·79	56·79	58·30	60·51	63·91								
0·70	R	33·79	33·80	33·82	33·85	33·90	34·04	34·26	34·59	35·17	36·99							
	UR	55·26	55·31	55·44	55·65	55·97	56·89	58·26	60·22	63·05	68·05							
0·75	R	31·09	31·09	31·11	31·13	31·17	31·29	31·46	31·71	32·09	32·84							
	UR	55·72	55·76	55·89	56·09	56·38	57·23	58·50	60·27	62·75	66·42							
0·80	R	27·90	27·90	27·92	27·96	27·97	28·06	28·20	28·39	28·67	29·11	30·55						
	UR	56·17	56·21	56·33	56·52	56·79	57·60	58·78	60·42	62·67	65·81	71·16						
0·85	R	24·28	24·28	24·30	24·31	24·34	24·42	24·54	24·69	24·91	25·21	25·75						
	UR	56·69	56·73	56·84	57·02	57·29	58·06	59·17	60·72	62·80	65·63	69·74						
0·90	R	19·86	19·86	19·87	19·88	19·90	19·97	20·06	20·18	20·34	20·56	20·87	20·82					
	UR	57·26	57·30	57·41	57·58	57·83	58·57	59·64	61·11	63·07	65·70	69·34	75·41					
0·95	R	13·58	13·58	13·59	13·60	13·62	13·66	13·72	13·81	13·92	14·06	14·24	14·53					
	UR	57·82	57·86	57·96	58·13	58·37	59·09	60·12	61·54	63·42	65·90	69·27	74·22					
1·00	R	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00					
	UR	58·60	58·40	58·50	58·66	58·91	59·60	60·61	61·98	63·80	66·19	69·39	74·94					

Table 2. Overall value $\overline{R(I)}$ (in %) as a function of σ_{1c}^2 and σ_1^2 for the related and unrelated cases a non-centrosymmetric crystal with a centrosymmetric group in the unit cell.

σ_1^2 ↓ \ σ_{1c}^2 →		0·00	0·05	0·10	0·15	0·20	0·30	0·40	0·50	0·60	0·70	0·80	0·90
0·00	R	100·00											
	UR	100·00											
0·05	R	95·44	95·58										
	UR	95·48	95·69										
0·10	R	91·53	91·62	91·90									
	UR	91·82	92·01	92·58									
0·15	R	88·05	88·10	88·27	88·59								
	UR	88·91	89·08	89·60	90·45								
0·20	R	84·83	84·86	84·95	85·13	85·43							
	UR	86·64	86·79	87·25	88·01	89·10							
0·25	R	81·86	81·88	81·92	82·01	82·17							
	UR	85·03	85·17	85·58	86·27	87·26							
0·30	R	78·85	78·86	78·87	78·91	78·97	79·32						
	UR	83·79	83·91	84·29	84·92	85·81	88·44						
0·35	R	76·07	76·07	76·06	76·06	76·07	76·18						
	UR	83·20	83·31	83·66	84·23	85·05	87·44						
0·40	R	73·16	73·16	73·14	73·11	73·08	73·04	73·20					
	UR	82·91	83·02	83·34	83·87	84·62	86·82	90·04					
0·45	R	70·01	70·00	69·98	69·95	69·91	69·80	69·75					
	UR	82·81	82·91	83·21	83·71	84·41	86·46	89·43					
0·50	R	67·14	67·13	67·11	67·07	67·01	66·86	66·70	66·68				
	UR	83·37	83·46	83·74	84·21	84·86	86·77	89·51	93·22				
0·55	R	63·94	63·93	63·91	63·86	63·80	63·62	63·39	63·18				
	UR	84·09	84·17	84·44	84·88	85·50	87·28	89·85	93·28				

0·60	R	60·54	60·53	60·50	60·45	60·38	60·18	59·91	59·59	59·36			
	UR	85·07	85·15	85·40	85·82	86·40	88·09	90·51	93·71	97·84			
0·65	R	56·57	56·56	56·53	56·48	56·41	56·21	55·93	55·57	55·20			
	UR	86·11	86·19	86·43	86·83	87·38	89·00	91·29	94·32	98·17			
0·70	R	52·75	52·74	52·71	52·67	52·62	52·45	52·21	51·89	51·51	51·17		
	UR	87·54	87·61	87·84	88·22	88·76	90·30	92·50	95·37	99·01	103·53		
0·75	R	48·83	48·83	48·80	48·76	48·71	48·55	48·33	48·03	47·65	47·21		
	UR	89·38	89·45	89·67	90·04	90·55	92·02	94·11	96·85	100·28	104·52		
0·80	R	43·99	43·98	43·96	43·92	43·87	43·73	43·52	43·25	42·89	42·45	41·98	
	UR	91·22	91·29	91·50	91·86	92·35	93·77	95·78	98·40	101·68	105·69	110·57	
0·85	R	38·39	38·39	38·37	38·34	38·31	38·19	38·02	37·80	37·50	37·12	36·64	
	UR	93·22	93·29	93·50	93·84	94·32	95·69	97·63	100·16	103·31	107·13	111·74	
0·90	R	31·34	31·34	31·33	31·30	31·27	31·18	31·04	30·85	30·60	30·29	29·87	29·34
	UR	95·35	95·42	95·61	95·95	96·41	97·74	99·62	102·06	105·10	108·78	113·18	118·43
0·95	R	20·96	20·95	20·94	20·93	20·90	20·83	20·72	20·58	20·39	20·15	19·83	19·40
	UR	97·48	97·54	97·74	98·06	98·51	99·81	101·64	104·01	106·97	110·53	114·76	119·77
1·00	R	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00
	UR	100·00	99·66	99·85	100·17	100·61	101·88	103·67	106·00	108·88	112·35	116·47	121·29

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