Acta Cryst. (1993). A49, 162-170

Statistical Characteristics of the Truncated Wilson Distributions

BY S. PARTHASARATHY* AND K. SEKAR

Department of Crystallography and Biophysics,† *University of Madras, Guindy Campus, Madras* 600025, *India*

(*Received* 8 *January* 1992; *accepted* 24 *June* 1992)

Abstract

Theoretical expressions are derived for $\langle y^n\rangle$, $n=1$ to 8, $\langle(z-1)^n\rangle$, $n=2, 3$ and 4, $\langle(z-\langle z\rangle)^n\rangle$, $n=2, 3$ and 4, $\langle|z-1|\rangle$, $\langle|z-1|^3\rangle$ and $\langle|z-\langle z\rangle|^3\rangle$, where y is the normalized structure-factor magnitude and z $(=I/\langle I\rangle)$ is the normalized intensity, valid for the centric and acentric Wilson distributions truncated such that $a^{1/2}\le y\le b^{1/2}$. The final results are given in the form of a convenient table of expressions. The tests of the theoretical results using the observed intensity data of a few crystals show that the agreement between the experimental and the corresponding theoretical values obtained from the present theoretical results is better than the agreement with the values obtained from *MULTAN*80 in centrosymmetric structures, while the present theory and *MULTAN*80 are found to yield results that are equally good for non-centrosymmetric structures.

1. Introduction

An essential and useful step in crystal-structure analysis is the determination of the space-group symmetry of the crystal. The acentric and centric Wilson distributions‡ (Wilson, 1949) play a central role in this regard. The utility of these distributions lies in their applicability to crystals of all space groups provided there are a sufficiently large number of similar atoms in the asymmetric unit at random positions. The intensity data of a majority of organic crystal structures obey reasonably well the acentric or the centric Wilson distribution if the crystal is respectively non-centrosymmetric or centrosymmetric. In view of this, the standard structure-solution programs (*e.g.* *MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) list the experimental values of the statistical quantities $\langle y\rangle$, $\langle y^2\rangle$, $\langle y^3\rangle$, $\langle y^4\rangle$, $\langle y^5\rangle$, $\langle y^6\rangle$, $\langle|y^2-1|\rangle$, $\langle(y^2-1)^2\rangle$, $\langle(y^2-1)^3\rangle$ and $\langle|y^2-1|^3\rangle$ (where y is the normalized structure-factor magnitude) and their corresponding theoretical values for the acentric and centric Wilson distributions for comparison. These theoretical values pertain to the untruncated Wilson distributions (*i.e.* $0\le y<\infty$). However, the data of actual crystals are always truncated at the lower end of the intensity scale owing to 'unobserved reflections'. Furthermore, in connection with the higher-moment tests for space-group determination, Foster & Hargreaves (1963) noted that the experimental values of the higher moments of intensities are generally larger than the corresponding theoretically expected values. Similar features were also observed in the experimental values of $\langle y^4\rangle$, $\langle y^5\rangle$, $\langle y^6\rangle$ and $\langle|y^2-1|^3\rangle$ in the *MULTAN*80 outputs (Main *et al.*, 1980) of a few structures that we determined. One reason for this could be overestimation of the y values of a few of the very strong reflections. This implies that better agreement between the observed and the corresponding theoretical values of the various statistical quantities could be obtained by computing the experimental values of the moments by excluding a few largest y values‡ and comparing the experimental values thus obtained with their corresponding theoretical values computed for the appropriately truncated Wilson distributions. In this paper we shall therefore derive the theoretical expressions for $\langle y\rangle$, $\langle y^2\rangle$, $\langle y^3\rangle$, $\langle y^4\rangle$, $\langle y^5\rangle$, $\langle y^6\rangle$, $\langle|y^2-1|\rangle$, $\langle(y^2-1)^2\rangle$, $\langle(y^2-1)^3\rangle$, $\langle|y^2-1|^3\rangle$ applicable to the untruncated data $a^{1/2}\le y\le b^{1/2}$.

Following the usual notation used in the literature on statistical tests for centrosymmetry we shall use y in the place of the normalized structure-factor magnitude E used in direct-methods literature. The quantity y is related to the normalized intensity z and the intensity I as

$$y^2=z=I/\langle I\rangle, \tag{1}$$

where $\langle I\rangle$ is the local average value of I for reflections in a narrow region of $(\sin\theta)/\lambda$. From (1), the expectation value of any function $g(y)$ of y may be written as

$$\langle g(y)\rangle=\langle g(z^{1/2})\rangle. \tag{2}$$

* To whom correspondence should be addressed.

† Contribution No. 796.

‡ These are derived based on the central-limit theorem and are not valid in the presence of extreme heterogeneity and pseudosymmetry. These extreme situations are beyond the scope of the present paper. The approach of Shmueli and coworkers may be used to derive the exact distributions for such situations (see, for example, Weiss, Shmueli, Kiefer & Wilson, 1985; Shmueli, Weiss & Kiefer, 1985).

‡ These could be identified and excluded by the statistical procedure suggested in § 6.

0108-7673/93/010162-09$06.00

From (2) it is clear that the theoretical expressions for $\langle g(y)\rangle$ may be derived by making use of the p.d.f. (probability density function) of z. Since it is more convenient to use z instead of y, we shall generally use the variable z in the theoretical derivations. For similar reasons we shall use the quantities $\langle(z-1)^2\rangle$, $\langle|z-1|^3\rangle$ *etc.* instead of the equivalent quantities $\langle(y^2-1)^2\rangle$, $\langle|y^2-1|^3\rangle$ *etc.*

Although $\langle z\rangle = 1$ for both acentric and centric Wilson distributions $(0\le z<\infty)$, $\langle z\rangle_t$ $(=M_1$, say) differs from unity for the truncated Wilson distributions (*i.e.* $a\le z\le b$) (see § 2 for notation). Hence quantities such as $\langle(z-1)^n\rangle$ and $\langle(z-M_1)^n\rangle$ will in general be different. Therefore, we shall also derive theoretical expressions for $\langle|z-M_1|^n\rangle$, $n=1,2,3$, in this paper. Since Srinivasan & Subramanian (1964) have shown that the theoretical values of $\langle y^8\rangle$ differ markedly for the centrosymmetric and noncentrosymmetric cases, we shall also derive theoretical expressions for $\langle y^7\rangle_t$ and $\langle y^8\rangle_t$ and in addition $\langle(z-1)^4\rangle_t$ and $\langle(z-M_1)^4\rangle_t$. The theoretical results reported in this paper were tested for a few crystal structures and the details of the results obtained are also presented here.

2. Notation, nomenclature and some preliminary results

We shall denote the intervals $0\le z<\infty$ and $a\le z\le b$ by the symbols Z and Z_t, respectively, and the intervals $0\le y<\infty$ and $a^{1/2}\le y\le b^{1/2}$ by Y and Y_t, respectively. We shall use t as a subscript to quantities that pertain to truncated distributions. For example, $P_t(z)$ is the p.d.f. of z for the truncated distribution defined in the interval Z_t, while $P(z)$ is the p.d.f. of z defined in the interval Z. It is convenient to use the abbreviations AWD, CWD, TAWD and TCWD for the acentric Wilson distribution, the centric Wilson distribution, the truncated acentric Wilson distribution and the truncated centric Wilson distribution, respectively. We shall refer to the distributions TAWD and TCWD together by the common symbol TWD (=truncated Wilson distributions) and the distributions AWD and CWD together by the common symbol WD (=Wilson distributions). We shall also use the symbols C and NC to stand for the centrosymmetric and noncentrosymmetric cases, respectively. It is convenient to define A_1 and A_2 by

$$\begin{aligned} A_1 &= 1/[\exp(-a)-\exp(-b)], \\ A_2 &= 1/[\operatorname{erf}(b^{1/2}/2^{1/2})-\operatorname{erf}(a^{1/2}/2^{1/2})]. \end{aligned} \tag{3}$$

The following results involving incomplete γ functions are needed in the theoretical simplifications and these can be derived easily from the recurrence relations of the γ function (Abramowitz & Stegun, 1965):

$$\gamma(1,x)=1-\exp(-x) \tag{4a}$$

$$\gamma(2,x)=1-(x+1)\exp(-x) \tag{4b}$$

$$\gamma(3,x)=2-(x^2+2x+2)\exp(-x) \tag{4c}$$

$$\gamma(4,x)=6-(x^3+3x^2+6x+6)\exp(-x) \tag{4d}$$

$$\gamma(5,x)=24-(x^4+4x^3+12x^2+24x+24)\exp(-x) \tag{4e}$$

$$\gamma(\tfrac{1}{2},x)=\pi^{1/2}\operatorname{erf}(x^{1/2}) \tag{5a}$$

$$\gamma(\tfrac{1}{2},x^2)=\pi^{1/2}\operatorname{erf}(x) \tag{5b}$$

$$\gamma(\tfrac{3}{2},x)=(\pi^{1/2}/2)\operatorname{erf}(x^{1/2})-x^{1/2}\exp(-x) \tag{5c}$$

$$\gamma(\tfrac{5}{2},x)=(3\pi^{1/2}/4)\operatorname{erf}(x^{1/2})-(x^{1/2}2)\times(2x+3)\exp(-x) \tag{5d}$$

$$\gamma(\tfrac{7}{2},x)=(15\pi^{1/2}/8)\operatorname{erf}(x^{1/2})-(x^{1/2}/4)\times(4x^2+10x+15)\exp(-x) \tag{5e}$$

$$\gamma(\tfrac{9}{2},x)=(105\pi^{1/2}/16)\operatorname{erf}(x^{1/2})-(x^{1/2}/8)(8x^3+28x^2+70x+105)\times\exp(-x). \tag{5f}$$

2.1. *Symbol for change in function value and its algebraic properties*

We shall use the notation $[f(x)]_p^q$ to stand for the change in the value of the function $f(x)$ as x changes its value from p to q,

$$[f(x)]_p^q=f(q)-f(p). \tag{6a}$$

We shall refer to the symbol $[f(x)]_a^b$ as the symbol for the change in the function value (SCFV hereafter). The following algebraic properties of the SCFV are extensively used in the theoretical simplifications:

$$[k_1]_a^b=0, \tag{6b}$$

$$[f(x)]_b^a=-[f(x)]_a^b, \tag{6c}$$

$$[f(x)]_a^b+[f(x)]_b^c=[f(x)]_a^c, \tag{6d}$$

$$[k_1+k_2f(x)]_a^b=k_2[f(x)]_a^b, \tag{6e}$$

$$[k_1f(x)+k_2g(x)]_a^b=k_1[f(x)]_a^b+k_2[g(x)]_a^b, \tag{6f}$$

$$k_1[k_2+k_3f(x)]_a^b+k_4[k_5+k_6g(x)]_a^b=[k_1k_3f(x)+k_4k_6g(x)]_a^b, \tag{6g}$$

where the k_i are constants. Using the notation for the SCFV, we can rewrite (3) as

$$A_1=1/[-\exp(-x)]_a^b, \qquad A_2=1/[\operatorname{erf}(x^{1/2}/2^{1/2})]_a^b.$$

In § 3 we shall derive some general theoretical results that are needed to derive the truncated Wilson distributions and the moments of z and $|z-c|$ (where c is a constant) for these distributions. These results are used to obtain results pertaining to the TAWD and the TCWD in §§ 4 and 5, respectively. Tests of the theoretical results for a few cases are given in § 6.

3. Derivation of theoretical results for any truncated distribution

3.1. *Theoretical formulae for the p.d.f.*

Let $P(z)$ and $N(z)$ be respectively the p.d.f. and cumulative function (c.f. hereafter) of a random variable z* defined in the interval $0 \leq z < \infty$. Let $P_t(z)$ and $N_t(z)$ be respectively the p.d.f. and c.f. of z when the data is truncated such that $a \leq z \leq b$. The p.d.f. of z for the truncated distribution can be obtained from that of the corresponding untruncated distribution by using the result (Eadie, Drijard, James, Roos & Saadoulet, 1972)

$$P_t(z) = P(z)/[N(b) - N(a)], \qquad z \in Z_t. \tag{7}$$

The cumulative function of z for the truncated distribution can be obtained from that of the untruncated distribution as

$$N_t(z) = [N(z) - N(a)]/[N(b) - N(a)], \qquad z \in Z_t. \tag{8}$$

3.2. *Theoretical formula for $\langle (z-c)^n \rangle$*

The nth moment of z about $z = c$ (where c is a constant) for the truncated distribution is given by

$$\begin{aligned}\langle (z-c)^n \rangle_t &= \left\langle \sum_{k=0}^{n} \binom{n}{k} (-c)^{n-k} z^k \right\rangle_t \\ &= \sum_{k=0}^{n} \binom{n}{k} (-c)^{n-k} \langle z^k \rangle_t,\end{aligned} \tag{9}$$

where we have used the binomial theorem for an integral exponent to expand $(z-c)^n$ and also the linearity property of the expectation value. Let M_k stand for the kth moment of z about the origin for the truncated distribution,

$$M_k = \langle z^k \rangle_t = \int_a^b z^k P_t(z)\,\mathrm{d}z. \tag{10}$$

From (10) we can rewrite (9) as

$$\langle (z-c)^n \rangle_t = \sum_{k=0}^{n} \binom{n}{k} (-c)^{n-k} M_k. \tag{11}$$

3.3. *Theoretical formula for $\langle |z-c|^n \rangle$*

We shall consider the following two cases: (i) $c = 1$ and (ii) $c = M_1$. When n is even ($=2m$, say), we have

$$\langle |z-c|^{2m} \rangle_t = \langle (z-c)^{2m} \rangle_t, \tag{12}$$

which may be evaluated using (11). The evaluation of odd-order moments of $|z-1|$ is more complicated and we shall presently consider this aspect. The method of derivation differs for the following two situations: (i) $a < 1 < b$ and (ii) $1 < a < b$. The former situation is the one generally met with in statistical tests for centrosymmetry. The latter situation arises when we compute the theoretical values of the odd-order moments of $|z-1|$ using data in which $z > 1$. For the sake of completeness we shall also consider this situation.

3.3.1. *Expression for $\langle |z-1|^{2n+1} \rangle_t$ for the situation in which $a < 1 < b$.* The $(2n+1)$th moment of $|z-1|$ for the truncated distribution is given by

$$\langle |z-1|^{2n+1} \rangle_t = \int_a^b |z-1|^{2n+1} P_t(z)\,\mathrm{d}z. \tag{13}$$

Clearly, we have

$$\begin{aligned}|z-1| &= 1 - z = -(z-1) \qquad &\text{for } z < 1 \\ &= z - 1 &\text{for } z \geq 1.\end{aligned} \tag{14}$$

Moreover, we can write

$$\int_a^b |z-1|^{2n+1} P_t(z)\,\mathrm{d}z = \int_a^1 |z-1|^{2n+1} P_t(z)\,\mathrm{d}z + \int_1^b |z-1|^{2n+1} P_t(z)\,\mathrm{d}z. \tag{15}$$

In view of (14) and (15), we can rewrite (13) as

$$\langle |z-1|^{2n+1} \rangle_t = -\int_a^1 (z-1)^{2n+1} P_t(z)\,\mathrm{d}z + \int_1^b (z-1)^{2n+1} P_t(z)\,\mathrm{d}z. \tag{16}$$

Since

$$\int_1^b (z-1)^{2n+1} P_t(z)\,\mathrm{d}z = \int_a^b (z-1)^{2n+1} P_t(z)\,\mathrm{d}z - \int_a^1 (z-1)^{2n+1} P_t(z)\,\mathrm{d}z,$$

we can rewrite (16) as

$$\langle |z-1|^{2n+1} \rangle_t = \langle (z-1)^{2n+1} \rangle_t - 2 \int_a^1 (z-1)^{2n+1} P_t(z)\,\mathrm{d}z. \tag{17}$$

Expanding $(z-1)^{2n+1}$ of the second term on the right-hand side of (17) by using the binomial theorem and interchanging the order of summation and integration, we obtain

$$\langle |z-1|^{2n+1} \rangle_t = \langle (z-1)^{2n+1} \rangle_t - 2 \sum_{k=0}^{2n+1} (-1)^{2n-k+1} \times \binom{2n+1}{k} \int_a^1 z^k P_t(z)\,\mathrm{d}z. \tag{18}$$

---

* The results in § 3 are applicable not only to the normalized intensity variable z but also to any random variable defined originally in the interval $(0, \infty)$, truncated to $[a, b]$.

3.3.2. *Expression for* $\langle|z-1|^{2n+1}\rangle_t$ *for the situation* $1<a<b$. For this case, $z>1$, so that $|z-1|=z-1$. Hence, we can write

$$\langle|z-1|^{2n+1}\rangle_t=\langle(z-1)^{2n+1}\rangle_t. \quad (19)$$

3.3.3. *Expression for* $\langle|z-M_1|^{2n+1}\rangle_t$. We know that $a<M_1<b$. Following the procedure used in § 3.3.1 we can easily show that

$$\langle|z-M_1|^{2n+1}\rangle_t=\langle(z-M_1)^{2n+1}\rangle_t -2\int_a^{M_1}(z-M_1)^{2n+1}P_t(z)\,dz. \quad (20)$$

Following the procedure used to obtain (18) from (17), we can obtain from (20) the expression

$$\langle|z-M_1|^{2n+1}\rangle_t=\langle(z-M_1)^{2n+1}\rangle_t-2\sum_{k=0}^{2n+1}(-M_1)^{2n-k+1} \times\binom{2n+1}{k}\int_a^{M_1}z^kP_t(z)\,dz. \quad (21)$$

4. Derivation of the theoretical expressions for the TAWD

4.1. *Expressions for the p.d.f. and c.f. of z and y*

The p.d.f. and c.f. of z for the AWD are known to be (Srinivasan & Parthasarathy, 1976; SP76 hereafter)

$$P(z)=\exp(-z), \qquad 0\le z<\infty, \quad (22)$$

$$N(z)=1-\exp(-z), \qquad 0\le z<\infty. \quad (23)$$

Using (22) and (23) in (7), we obtain the p.d.f. of z for the TAWD as

$$P_t(z)=A_1\exp(-z), \qquad z\in Z_t, \quad (24)$$

where A_1 is as defined in (3). Using (23) in (8), we obtain the c.f. of z for the TAWD to be

$$N_t(z)=A_1[\exp(-a)-\exp(-z)], \qquad z\in Z_t. \quad (25)$$

Making use of (7) and (8) and the p.d.f. and c.f. of y for AWD available in SP76, we can obtain the p.d.f. and c.f. of y for the TAWD,

$$P_t(y)=2A_1y\exp(-y^2), \qquad y\in Y_t, \quad (26)$$

$$N_t(y)=A_1[\exp(-a)-\exp(-y^2)], \qquad y\in Y_t. \quad (27)$$

4.2. *Expressions for* $\langle z^n\rangle_t$ *and* $\langle y^{2n+1}\rangle$, $n=1,2,3,4$

It may be seen from (10) that, for the TAWD,

$$M_0=1, \quad (28)$$

which is the normalization condition for $P_t(z)$. Making use of (24) in (10), we obtain the nth moment of z for the TAWD,

$$\langle z^n\rangle_t=A_1\int_a^b z^n\exp(-z)\,dz=A_1[\gamma(n+1,x)]_a^b = M_n, \quad \text{say}. \quad (29)$$

Making use of (4b) to (4e) in (29), we can derive explicit expressions for the first four moments of z; these are given in rows 5, 6, 7 and 8 of Table 1.

From (29) we obtain the nth moment of y,

$$\langle y^n\rangle_t=\langle z^{n/2}\rangle_t=A_1[\gamma(n/2+1,x)]_a^b. \quad (30)$$

Making use of (5c) to (5f) in (30), we can obtain explicit expressions for the first four odd moments of y; these are given in rows 1, 2, 3 and 4 of Table 1.

4.3. *Expressions for* $\langle(z-1)^n\rangle_t$ *and* $\langle(z-M_1)^n\rangle_t$, $n=2,3,4$

Making use of (29) in (11) and then carrying out some algebraic manipulations using the properties of the SCFV, we can show that

$$\langle(z-1)^n\rangle_t=A_1\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}[\gamma(k+1,x)]_a^b. \quad (31)$$

Putting $n=2$, 3 and 4 successively in (31), using (4a) to (4e) and the properties of SCFV, we can derive explicit expressions for the second, third and fourth moments of $z-1$; these are given in rows 9, 10 and 11 of Table 1.

Making use of (29) in (11) and then carrying out some algebraic manipulations using the properties of the SCFV, we can show that

$$\langle(z-M_1)^n\rangle_t=A_1\sum_{k=0}^{n}\binom{n}{k}(-M_1)^{n-k}[\gamma(k+1,x)]_a^b. \quad (32)$$

Putting $n=2$, 3 and 4 successively in (32), using (4a) to (4e) and the properties of the SCFV, we can derive explicit expressions for the second, third and fourth moments of $z-M_1$; these are given in rows 15 and 16 of Table 1. It may be noted that $\langle(z-M_1)^2\rangle_t$ is the variance of z.

4.4. *Expressions for* $\langle|z-1|^{2n+1}\rangle_t$, $n=0,1$

4.4.1. *Results for the situation* $a<1<b$. Using (24) in (18), we obtain

$$\langle|z-1|^{2n+1}\rangle_t=\langle(z-1)^{2n+1}\rangle_t-2A_1\sum_{k=0}^{2n+1}(-1)^{2n-k+1} \times\binom{2n+1}{k}[\gamma(k+1,x)]_a^1. \quad (33)$$

Putting $n=0$ and 1 successfully in (33), using (4a) to (4e) and the properties of the SCFV, we can derive expressions for the first and third moments of $|z-1|$ and these are given in rows 12 and 13 of Table 1.

Table 1. *Summary of statistical characteristics of the TAWD and TCWD*

No.	Statistical characteristic	Theoretical expression for TAWD	Theoretical expression for TCWD
1	$\langle y\rangle_t$	$A_1[(\pi^{1/2}/2)\,\mathrm{erf}\,(x^{1/2})-x^{1/2}\exp(-x)]_a^b$	$(2^{1/2}/\pi^{1/2})A_2[(\exp(-x)]_{b/2}^{a/2}$
2	$\langle y^3\rangle_t$	$A_1[(3\pi^{1/2}/4)\,\mathrm{erf}\,(x^{1/2})-(x^{1/2}/2)(2x+3)\exp(-x)]_a^b$	$2(2^{1/2}/\pi^{1/2})A_2[(x+1)\exp(-x)]_{b/2}^{a/2}$
3	$\langle y^5\rangle_t$	$A_1[(15\pi^{1/2}/8)\,\mathrm{erf}\,(x^{1/2})-(x^{1/2}/4)(4x^2+10x+15)\exp(-x)]_a^b$	$4(2^{1/2}/\pi^{1/2})A_2[(x^2+2x+2)\exp(-x)]_{b/2}^{a/2}$
4	$\langle y^7\rangle_t$	$A_1[(105\pi^{1/2}/16)\,\mathrm{erf}\,(x^{1/2})-(x^{1/2}/8)$ $\times(8x^3+28x^2+70x+105)\exp(-x)]_a^b$	$8(2^{1/2}/\pi^{1/2})A_2[(x^3+3x^2+6x+6)\exp(-x)]_{b/2}^{a/2}$
5	$\langle z\rangle_t=M_1$	$1-A_1[x\exp(-x)]_a^b$	$1-(2/\pi^{1/2})A_2[x^{1/2}\exp(-x)]_{a/2}^{b/2}$
6	$\langle z^2\rangle_t$	$2-A_1[x(x+2)\exp(-x)]_a^b$	$3-(2/\pi^{1/2})A_2[x^{1/2}(2x+3)\exp(--x)]_{a/2}^{b/2}$
7	$\langle z^3\rangle_t$	$6-A_1[x(x^2+3x+6)\exp(-x)]_a^b$	$15-(2/\pi^{1/2})A_2[x^{1/2}(4x^2+10x+15)\exp(-x)]_{a/2}^{b/2}$
8	$\langle z^4\rangle_t$	$24-A_1[x(x^3+4x^2+12x+24)\exp(-x)]_a^b$	$105-(2/\pi^{1/2})A_2[x^{1/2}(8x^3+28x^2+70x+105)\exp(-x)]_{a/2}^{b/2}$
9	$\langle(z-1)^2\rangle_t$	$1-A_1[x^2\exp(-x)]_a^b$	$2-(2/\pi^{1/2})A_2[x^{1/2}(2x+1)\exp(-x)]_{a/2}^{b/2}$
10	$\langle(z-1)^3\rangle_t$	$2-A_1[x(x^2+3)\exp(-x)]_a^b$	$8-(2/\pi^{1/2})A_2[x^{1/2}(4x^2+4x+9)\exp(-x)]_{a/2}^{b/2}$
11	$\langle(z-1)^4\rangle_t$	$9-A_1[x(x^3+6x+8)\exp(-x)]_a^b$	$60-(2/\pi^{1/2})A_2[x^{1/2}(8x^3+12x^2+42x+59)\exp(-x)]_{a/2}^{b/2}$
12	$\langle\lvert z-1\rvert\rangle_t$	(i) $A_1[2\exp(-1)-a\exp(-a)-b\exp(-b)]$ if $a<1<b$	$(2/\pi^{1/2})A_2\{[x^{1/2}\exp(-x)]_{a/2}^{1/2}+[x^{1/2}\exp(-x)]_{b/2}^{1/2}\}$ if $a<1<b$
		(ii) $A_1[x\exp(-x)]_b^a$ if $1<a<b$	$(2/\pi^{1/2})A_2[x^{1/2}\exp(-x)]_{b/2}^{a/2}$ if $1<a<b$
13	$\langle\lvert z-1\rvert^3\rangle$	(i) $2+A_1[12\exp(-1)-(a^3+3a+4)\exp(-a)$ $-(b^3+3b)\exp(-b)]$ if $a<1<b$	$8-(2/\pi^{1/2})A_2[x^{1/2}(4x^2+4x+9)\exp(-x)]_{a/2}^{b/2}$ $-16A_2[\mathrm{erf}\,(x^{1/2})]_{a/2}^{1/2}$ $+\pi^{-1/2}A_2[(16x^2+16x+36)x^{1/2}\exp(-x)]_{a/2}^{1/2}$ if $a<1<b$
		(ii) $2-A_1[x(x^2+3)\exp(-x)]_a^b$ if $1<a<b$	$8-(2/\pi^{1/2})A_2[x^{1/2}(4x^2+4x+9)\exp(-x)]_{a/2}^{b/2}$ if $1<a<b$
14	$\langle(z-M_1)^2\rangle_t$	$(M_1^2-2M_1+2)-A_1[x(x-2M_1+2)\exp(-x)]_a^b$	$(M_1^2-2M_1+3)-(2/\pi^{1/2})A_2[x^{1/2}\exp(-x)$ $\times(2x+3-2M_1)]_{a/2}^{b/2}$
15	$\langle(z-M_1)^3\rangle_t$	$(6-6M_1+3M_1^2-M_1^3)-A_1[x\{x^2-3(M_1-1)x$ $+3(M_1^2-2M_1+2)\}\exp(-x)]_a^b$	$15-9M_1+3M_1^2-M_1^3-(2/\pi^{1/2})A_2[x^{1/2}\exp(-x)$ $\times\{4x^2+(10-6M_1)x+(3M_1^2-9M_1+15)\}]_{a/2}^{b/2}$
16	$\langle(z-M_1)^4\rangle_t$	$24-24M_1+12M_1^2-4M_1^3+M_1^4$ $-A_1[x\{x^3-4(1-M_1)x^2+6x(2-2M_1+M_1^2)$ $+4(6-6M_1+3M_1^2-M_1^3)\}\exp(-x)]_a^b$	$105-60M_1+18M_1^2-4M_1^3+M_1^4$ $-(2/\pi^{1/2})A_2[\{8x^3+(28-16M_1)x^2$ $+(70-40M_1+12M_1^2)x$ $+(105-60M_1+18M_1^2-4M_1^3)\}x^{1/2}\exp(-x)]_{a/2}^{b/2}$
17	$\langle\lvert z-M_1\rvert\rangle_t$	$2A_1[(1-M_1+x)\exp(-x)]_a^{M_1}$	$A_2\{2(M_1-1)[\mathrm{erf}\,(x^{1/2})]_{a/2}^{M_1/2}+(4/\pi^{1/2})$ $\times[x^{1/2}\exp(-x)]_{a/2}^{M_1/2}\}$
18	$\langle\lvert z-M_1\rvert^3\rangle_t$	$6-6M_1+3M_1^2-M_1^3-A_1[\{x^3-3(M_1-1)x^2$ $+3(M_1^2-2M_1+2)x\}\exp(-x)]_a^b$ $-2A_1[\{M_1^3-3M_1^2+6M_1-6-3(M_1^2-2M_1+2)x$ $+3(M_1-1)x^2-x^3\}\exp(-x)]_a^{M_1}$	$(M_1^3-3M_1^2+9M_1-15)\{2A_2[\mathrm{erf}(x^{1/2})]_{a/2}^{M_1/2}-1\}$ $-(2/\pi^{1/2})A_2[\{4x^2+(10-6M_1)x$ $+(3M_1^2-9M_1+15)\}x^{1/2}\exp(-x)]_{a/2}^{b/2}$ $+(4/\pi^{1/2})A_2[\{4x^2+(10-6M_1)x$ $+(3M_1^2-9M_1+15)\}x^{1/2}\exp(-x)]_{a/2}^{M_1/2}$

4.4.2. *Results for the situation* $1<a<b$. Putting $n=0$ in (19) and using the expression for $\langle z\rangle_t$ from Table 1, we can obtain explicit expressions for $\langle|z-1|\rangle_t$. Putting $n=1$ in (19) and using the appropriate expression (row 10) in Table 1 for $\langle(z-1)^3\rangle$, we can obtain explicit expressions for $\langle|z-1|^3\rangle_t$. These expressions are given in rows 12 and 13 of Table 1.

4.5. *Expressions for* $\langle|z-M_1|^{2n+1}\rangle_t$, $n=0, 1$

Using (24) in (21), we obtain

$$\langle|z-M_1|^{2n+1}\rangle_t=\langle(z-M_1)^{2n+1}\rangle_t -2A_1\sum_{k=0}^{2n+1}\binom{2n+1}{k}(-M_1)^{2n-k+1} \times[\gamma(k+1,x)]_a^{M_1}. \tag{34}$$

Putting $n=0$, 1 and 2 successively in (34), simplifying the resulting expressions using ($4a$) to ($4e$) and using the properties of the SCFV, we can obtain explicit expressions for the first and third moments of $|z-M_1|$; these are given in rows 17 and 18 of Table 1.

5. Derivation of the theoretical values for the TCWD

5.1. *Expressions for the p.d.f. and c.f. of z and y*

Making use of (7) and (8) and the expressions for the p.d.f. and c.f. of z and y for the CWD in SP76, we obtain

$$P_t(z)=A_2(2\pi z)^{-1/2}\exp(-z/2), \qquad z\in Z_t, \tag{35}$$

$$N_t(z)=A_2[\mathrm{erf}\,(z^{1/2}/2^{1/2})-\mathrm{erf}\,(a^{1/2}/2^{1/2})], \qquad z\in Z_t, \tag{36}$$

$$P_t(y)=A_2(2/\pi)^{1/2}\exp(-y^2/2), \qquad y\in Y_t, \tag{37}$$

$$N_t(y)=A_2[\mathrm{erf}\,(y/2^{1/2})-\mathrm{erf}\,(a^{1/2}/2^{1/2})], \qquad y\in Y_t. \tag{38}$$

5.2. *Expressions for* $\langle z^n\rangle_t$ and $\langle y^{2n+1}\rangle_t$, $n=1, 2, 3, 4$

It may be seen from (10) that for the TCWD

$$M_0 = 1, \tag{39}$$

which is a consequence of the normalization of $P_t(z)$. Making use of (35), we obtain the nth moment of z,

$$M_n = A_2(2\pi)^{-1/2} \int_a^b z^{n-1/2} \exp(-z/2)\, dz. \tag{40}$$

Using the substitution $t = z/2$, we can rewrite (40) as

$$M_n = 2^n \pi^{-1/2} A_2[\gamma(n+\tfrac{1}{2}, x)]_{a/2}^{b/2}. \tag{41}$$

Making use of (5*c*) to (5*f*) in (41) and the properties of the SCFV we can derive explicit expressions for the first four moments of z; these are given in rows 5, 6, 7 and 8 of Table 1.

From (41) we obtain the nth moment of y to be

$$\begin{aligned}\langle y^n\rangle_t &= \langle z^{n/2}\rangle_t \\ &= 2^{n/2}\pi^{-1/2}A_2\{\gamma[(n+1)/2, x]\}_{a/2}^{b/2}.\end{aligned} \tag{42}$$

Making use of (4*a*) to (4*d*) in (42) and the properties of the SCFV we can derive the explicit expressions for the first four odd moments of y and these are given in rows 1, 2, 3 and 4 of Table 1.

5.3. *Expressions for* $\langle (z-1)^n\rangle_t$ *and* $\langle (z-M_1)^n\rangle_t$, $n=2,3,4$

Making use of (41) in (11), we obtain, after some algebraic manipulations using the properties of SCFV,

$$\langle (z-1)^n\rangle_t = \pi^{-1/2}A_2 \sum_{k=0}^{n} (-1)^{n-k}2^k \times \binom{n}{k}[\gamma(k+\tfrac{1}{2}, x)]_{a/2}^{b/2}. \tag{43}$$

Putting $n=2$, 3 and 4 successively in (43) and using (4*b*) and (5*b*) to (5*f*), we can derive explicit expressions for the second, third and fourth moments of $z-1$; these are given in rows 9, 10 and 11 of Table 1.

Making use of (41) in (11), we obtain, after carrying out some algebraic manipulations,

$$\langle (z-M_1)^n\rangle_t = \pi^{-1/2}A_2 \sum_{k=0}^{n} \binom{n}{k} (-M_1)^{n-k}2^k \times [\gamma(k+\tfrac{1}{2}, x)]_{a/2}^{b/2}. \tag{44}$$

Putting $n=2,3$ and 4 successively in (44) and using the properties of the SCFV we can derive explicit expressions for the second, third and fourth moments of $z-M_1$; these are given in rows 14, 15 and 16 of Table 1.

5.4. *Expressions for* $\langle |z-1|^{2n+1}\rangle_t$, $n=0, 1$

5.4.1. *Results for the situation* $a<1<b$. Making use of (35) in (18), we obtain

$$\begin{aligned}\langle |z-1|^{2n+1}\rangle_t &= \langle (z-1)^{2n+1}\rangle_t \\ &\quad -2(2\pi)^{-1/2}A_2 \sum_{k=0}^{2n+1} (-1)^{2n-k+1} \\ &\quad \times \binom{2n+1}{k} \int_a^1 z^{k-1/2}\exp(-z/2)\, dz.\end{aligned} \tag{45}$$

Substituting $z/2 = x$ in (45), we obtain

$$\begin{aligned}\langle |z-1|^{2n+1}\rangle_t &= \langle (z-1)^{2n+1}\rangle_t \\ &\quad -\pi^{-1/2}A_2 \sum_{k=0}^{2n+1} (-1)^{2n-k+1}2^{k+1} \\ &\quad \times \binom{2n+1}{k}[\gamma(k+\tfrac{1}{2}, x)]_{a/2}^{1/2}.\end{aligned} \tag{46}$$

Putting $n=0$ and 1 successively in (46) and using (5*a*) to (5*e*) and the properties of the SCFV, we can derive explicit expressions for the first and third moments of $\langle |z-1|\rangle$; these are given in rows 12 and 13 of Table 1.

5.4.2. *Results for the situation* $1<a<b$. Using (19) and the appropriate expressions $\langle z\rangle_t$ for $\langle (z-1)^3\rangle_t$ from row 1 of Table 1, we can obtain explicit expressions for $\langle |z-1|\rangle_t$ and $\langle |z-1|^3\rangle_t$; these are given in rows 12 and 13 of Table 1.

5.5. *Expressions for* $\langle |z-M_1|^{2n+1}\rangle_t$, $n=0, 1$

Using (35) in (21) we obtain

$$\begin{aligned}\langle |z-M_1|^{2n+1}\rangle_t &= \langle (z-M_1)^{2n+1}\rangle_t - 2^{1/2}\pi^{-1/2}A_2 \\ &\quad \times \sum_{k=0}^{2n+1} (-M_1)^{2n-k+1}\binom{2n+1}{k} \\ &\quad \times \int_a^{M_1} z^{k-1/2}\exp(-z/2)\, dz.\end{aligned} \tag{47}$$

Substituting $z/2 = x$, we can rewrite (47) as

$$\begin{aligned}\langle |z-M_1|^{2n+1}\rangle_t &= \langle (z-M_1)^{2n+1}\rangle_t - \pi^{-1/2}A_2 \\ &\quad \times \sum_{k=0}^{2n+1} (-M_1)^{2n-k+1}2^{k+1}\binom{2n+1}{k} \\ &\quad \times [\gamma(k+\tfrac{1}{2}, x)]_{a/2}^{M_1/2}.\end{aligned} \tag{48}$$

Putting $n=0$, 1 and 2 successively in (48) and then simplifying the resulting expressions using (5*a*) to (5*e*) and the properties of the SCFV, we can obtain explicit expressions for the first and third moments

Table 2. *Details of the crystals used in the statistical tests and related results*

n_1: total number of possible independent three-dimensional reflections in the interval $S_{\min} \leq (\sin\theta)/\lambda \leq S_{\max}$.
n_2: number of reflections, out of the n_1 reflections, for which $y < a^{1/2}$.
n_3: number of reflections, out of the n_1 reflections, for which $y > b^{1/2}$.
$p = 100(n_2 + n_3)/n_1$ = percentage of reflections, out of the n_1 reflections, that are not used in the test.

No.*	Molecular formula	Space group	$S_{\min}$	$S_{\max}$	$a^{1/2}$	$b^{1/2}$	n_1	n_2	n_3	p
1	$C_{20}H_{23}NO$	$P\bar{1}$	0.220	0.597	0.348	3.0	2210	563	12	26
2	$C_{20}H_{32}N_2O_3$	$P\bar{1}$	0.224	0.602	0.208	3.0	2878	459	11	16
3	$C_{22}H_{38}N_4O$	$P\bar{1}$	0.192	0.578	0.378	3.0	2789	791	15	29
4	$C_{13}H_{15}NO$	$P\bar{1}$	0.234	0.573	0.289	3.0	1148	259	11	24
5	$C_{17}H_{26}N_2O_3$	$P2_1/c$	0.193	0.579	0.279	3.0	2148	489	8	23
6	$C_{18}H_{19}NO$	$C2/c$	0.215	0.528	0.397	3.0	1347	420	6	32
7	$C_{24}H_{30}N_4O_2$	$I2/a$	0.174	0.526	0.376	3.0	2171	666	14	31
8	$C_{27}H_{34}O_5$	$P2_12_12_1$	0.210	0.550	0.527	2.5	1350	326	2	24
9	$C_{25}H_{28}O_8$	$P2_12_12_1$	0.228	0.546	0.546	2.9	1216	325	0	27

* References: (1) Sekar, Parthasarathy & Radhakrishnan (1993); (2) Shanmugasundarraj, Ponnuswamy, Shanmugam & Kandasamy (1992); (3) Velmurugan (1991); (4) Sekar, Parthasarathy, Prabahar & Ramakrishnan (1993); (5) Ponnuswamy & Kandasamy (1990); (6) Sekar, Parthasarathy & Rajalingam (1990); (7) Velmurugan (1992); (8) Sekar, Parthasarathy, Epe & Mondon (1992); Sekar, Parthasarathy, Epe & Mondon (1992).

of $|z - M_1|$; these are given in rows 17 and 18 of Table 1.

6. Test of the theoretical results

The theoretical results given in Table 1 were tested using the observed data of nine actual crystal structures. The observed *hkl* intensity data (corrected for Lorentz-polarization effects) on the same relative scale were used in calculating the experimental values of the various statistical parameters. The values of $a^{1/2}$ and $b^{1/2}$ are to be obtained for each crystal separately and the following procedure was used for this. The threshold value of y (*i.e.* y_t) due to the unobserved reflections, which can be determined from an analysis of the intensity data of the crystal as a function of $(\sin\theta)/\lambda$, was taken to be $a^{1/2}$. The value of $b^{1/2}$ for any given crystal may be obtained as follows: for crystals obeying the requirements of a WD only 0.3% of the reflections are expected to have y values greater than 3.0 for the centrosymmetric case and practically all the reflections are expected to have y values <3.0 for the noncentrosymmetric case (SP76). Hence, in an actual crystal containing similar atoms at general positions, if we find much more than 0.3% of reflections with $y > 3.0$, then it is most likely that some of the largest y values could have arisen due to overestimation. Hence we may set $b^{1/2} = 3.0$ if the y data of the crystal contains y values greater than 3.0. On the other hand, if the y data of the crystal is such that the maximum observed value of y is less than 3.0, then $b^{1/2}$ may be taken to be the largest observed value of y rounded off to one decimal place. The details of the crystals used in the statistical tests and the related results such as the values of $a^{1/2}$, $b^{1/2}$ and the percentage of reflections excluded from the test are given in Table 2. For each crystal the experimental y values were computed from the observed intensity data by using (1), the value of $\langle I\rangle$ for each reflection of the crystal being computed from the least-squares cubic-spline function (with smoothing) that fits $[(\sin\theta)/\lambda, \langle I\rangle]$ data.* The experimental and the corresponding theoretical values of the various statistical parameters for the nine crystals computed using the respective values of $a^{1/2}$ and $b^{1/2}$ thus obtained are given in Tables 3 and 4. Table 3 contains results for the statistical parameters that are listed in *MULTAN*80; Table 4 contains the results for the parameters not included in *MULTAN*80. A study of Tables 3 and 4 shows that there is reasonably good agreement between the observed and the corresponding theoretical values of the various statistical parameters. From Table 3 it is also seen that the agreement between the experimental and the corresponding theoretical values of higher moments obtained from the present theoretical results is better than the agreement with the *MULTAN*80 outputs for the centrosymmetric structures. In the case of the noncentrosymmetric structures, the present theory and *MULTAN*80 are found to yield results that are equally good. It may, however, be noted that the results obtained from *MULTAN*80 using $\langle y\rangle$ and $\langle y^3\rangle$ as test parameters are somewhat better than the results from the present theory. However, since the values of these parameters for centrosymmetric and noncentrosymmetric crystals are not very much different, they may not be very useful as statistical tests for centrosymmetry. The following incidental points may be noted: (i) Since $\langle y^2\rangle = 1$ for both CWD and AWD, it cannot be used as a parameter for testing for the centrosymmetry of the crystal, though it could be

* The actual computations of $a^{1/2}$, $b^{1/2}$ and y were done using the Fortran program *STATCW* (Sekar, 1991) developed by Parthasarathy and co-workers for conducting the various statistical tests for centrosymmetry. The details of *STATCW* will be published separately. *STATCW* is an improved version of *STATC* (Parthasarathy, Ponnuswamy, Elango & Sekar, 1990).

Table 3. *Theoretical and experimental values of* $\langle y^n \rangle$ $(n=1,2,\ldots,6)$, $\langle |z-1|^n \rangle$ $(n=1,3)$ *and* $\langle (z-1)^n \rangle$ $(n=2,3)$ *as obtained from MULTAN80 and STATCW for a few crystal structures*

A^*: theoretical value for AWD as obtained from *MULTAN*80.
E^*: experimental value as obtained from *MULTAN*80.
C^*: theoretical value for CWD as obtained from *MULTAN*80.
A: theoretical value for TAWD as obtained from the present theory.
E: experimental value as obtained from *STATCW*.
C: theoretical value for TCWD as obtained from the present theory.
$\langle (z-1)^2 \rangle$: variance of z.

No.	Space group		$\langle y \rangle$	$\langle y^2 \rangle$	$\langle y^3 \rangle$	$\langle y^4 \rangle$	$\langle y^5 \rangle$	$\langle y^6 \rangle$	$\langle \lvert z-1 \rvert \rangle$	$\langle (z-1)^2 \rangle$	$\langle (z-1)^3 \rangle$	$\langle \lvert z-1 \rvert^3 \rangle$
1	$P\bar{1}$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.795	0.996	1.665	3.405	8.066	21.288	0.984	2.414	13.059	13.741
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.970	1.120	1.494	2.243	3.706	6.628	0.708	1.003	2.259	2.512
		E	0.982	1.243	1.941	3.552	7.275	16.140	0.917	2.067	8.212	8.529
		C	1.023	1.323	2.062	3.683	7.271	15.453	0.938	2.037	7.373	7.659
2	$P\bar{1}$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.778	0.997	1.718	3.661	9.118	25.474	1.011	2.666	16.484	17.197
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.919	1.042	1.384	2.075	3.429	6.133	0.724	0.991	2.032	2.382
		E	0.885	1.080	1.664	3.005	6.040	13.081	0.921	1.846	6.305	6.796
		C	0.927	1.163	1.799	3.210	6.335	13.463	0.936	1.884	6.322	6.774
3	$P\bar{1}$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.779	0.996	1.713	3.761	10.340	35.045	1.044	2.770	25.748	26.455
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.984	1.141	1.526	2.292	3.787	6.774	0.705	1.009	2.323	2.553
		E	0.996	1.272	1.985	3.581	7.157	15.398	0.940	2.037	7.470	7.778
		C	1.004	1.361	2.126	3.801	7.504	15.947	0.940	2.078	7.629	7.883
4	$P\bar{1}$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.771	0.990	1.787	4.121	11.336	35.323	1.032	3.142	24.929	25.654
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.946	1.082	1.440	2.161	3.570	6.384	0.715	0.996	2.149	2.446
		E	0.912	1.115	1.727	3.161	6.471	14.302	0.914	1.931	7.165	7.581
		C	0.982	1.253	1.944	3.471	6.851	14.559	0.935	1.966	6.904	7.258
5	$P2_1/c$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.795	0.983	1.617	3.349	8.569	26.650	0.954	2.382	18.553	19.228
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.943	1.077	1.432	2.149	3.550	6.349	0.716	0.995	2.133	2.437
		E	0.962	1.207	1.848	3.261	6.373	13.446	0.919	1.846	6.286	6.665
		C	0.976	1.241	1.926	3.438	6.785	14.419	0.935	1.955	6.830	7.196
6	$C2/c$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.764	0.988	1.641	3.313	7.802	20.728	0.981	2.338	12.752	13.477
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.993	1.156	1.547	2.325	3.843	6.875	0.703	1.013	2.367	2.582
		E	1.033	1.332	2.074	3.727	7.432	16.001	0.924	2.062	7.818	8.065
		C	1.058	1.386	2.168	3.878	7.657	16.273	0.942	2.106	7.798	8.032
7	$I2/a$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.758	1.019	1.830	4.111	10.987	33.578	1.050	3.073	23.301	24.062
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	0.983	1.140	1.524	2.288	3.782	6.765	0.705	1.008	2.319	2.550
		E	1.002	1.286	2.024	3.706	7.556	16.643	0.936	2.134	8.383	8.681
		C	1.043	1.359	2.122	3.793	7.489	15.916	0.940	2.075	7.613	7.869
8	$P2_12_12_1$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.867	1.007	1.350	2.045	3.451	6.430	0.738	1.031	2.317	2.768
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	1.057	1.263	1.692	2.504	4.022	6.908	0.679	0.978	2.186	2.305
		E	1.048	1.240	1.648	2.428	3.906	6.754	0.659	0.948	2.189	2.307
		C	1.126	1.476	2.208	3.666	6.583	12.530	0.878	1.714	4.960	5.079
9	$P2_12_12_1$	A^*	0.886	1.000	1.329	2.000	3.323	6.000	0.736	1.000	2.000	2.415
		E^*	0.851	0.995	1.358	2.119	3.709	7.169	0.758	1.130	2.796	3.278
		C^*	0.798	1.000	1.596	3.000	6.383	15.000	0.968	2.000	8.000	8.691
		A	1.071	1.295	1.761	2.658	4.390	7.823	0.691	1.068	2.734	2.841
		E	1.070	1.301	1.796	2.793	4.837	9.197	0.698	1.191	3.722	3.829
		C	1.162	1.586	2.504	4.450	8.671	18.110	0.960	2.279	8.516	8.621

used to check the quality of the experimental data. (ii) In the case of any given crystal, if the experimental values of higher-order moments are highly enhanced compared with the corresponding theoretical values for the TWD, in spite of using the procedure suggested in this paper, then it would be reasonable to assume that these enhancements could have arisen from the violation of the basic requirements of the WD in such a crystal. The exact theoretical distributions required for such a crystal should then be obtained using the more rigorous treatment of Shmueli and co-workers (Shmueli, Weiss & Kiefer, 1985; Weiss, Shmueli,

Table 4. *Theoretical and experimental values of* $\langle y^7\rangle_t$, $\langle y^8\rangle_t$, $\langle (z-1)^4\rangle_t$, $\langle (z-M_1)^n\rangle_t$ ($n=2, 3$ *and* 4), $\langle |z-M_1|^n\rangle_t$ ($n=1$ *and* 3) *as obtained from STATCW for a few crystal structures*

A: theoretical values for TAWD as obtained from the present theory.
E: experimental values as obtained from *STATCW*.
C: theoretical values for TCWD as obtained from the present theory.
$\langle (z-M_1)^2\rangle$: variance of z for truncated distribution.

No.	Space group		$\langle y^7\rangle_t$	$\langle y^8\rangle_t$	$\langle (z-1)^4\rangle_t$	$\langle (z-M_1)^2\rangle_t$	$\langle (z-M_1)^3\rangle_t$	$\langle (z-M_1)^4\rangle_t$	$\langle \lvert z-M_1\rvert\rangle_t$	$\langle \lvert z-M_1\rvert^3\rangle_t$
1	$P\bar{1}$	A	12.66	25.59	9.06	0.989	1.902	8.06	0.734	2.315
		E	37.91	92.84	45.62	2.008	6.736	38.37	0.987	7.515
		C	34.72	81.45	37.44	1.932	5.465	29.15	1.012	6.376
2	$P\bar{1}$	A	11.71	23.68	8.43	0.990	1.907	8.10	0.734	2.320
		E	29.91	71.23	33.62	1.840	5.864	31.68	0.949	6.521
		C	30.25	70.95	32.71	1.857	5.410	28.89	0.983	6.207
3	$P\bar{1}$	A	12.94	26.16	9.25	0.989	1.901	8.05	0.734	2.314
		E	34.99	82.95	38.75	1.964	5.850	31.52	1.018	6.687
		C	35.83	84.05	38.62	1.947	5.471	29.17	1.018	6.406
4	$P\bar{1}$	A	12.20	24.65	8.75	0.989	1.905	8.08	0.734	2.318
		E	33.35	80.92	39.21	1.918	6.503	36.08	0.956	7.145
		C	32.71	76.73	35.31	1.902	5.447	29.08	1.000	6.310
5	$P2_1/c$	A	12.13	24.52	8.71	0.989	1.905	8.09	0.734	2.318
		E	30.07	70.37	32.32	1.803	5.156	27.58	0.972	5.950
		C	32.40	76.00	34.98	1.897	5.443	29.06	0.998	6.299
6	$C2/c$	A	13.13	26.55	9.38	0.989	1.900	8.04	0.734	2.313
		E	36.48	86.88	40.91	1.952	5.835	31.85	1.006	6.690
		C	36.56	85.77	39.40	1.956	5.474	29.17	1.022	6.424
7	$I2/a$	A	12.92	26.12	9.23	0.989	1.901	8.05	0.734	2.314
		E	38.80	94.42	45.94	2.053	6.601	37.38	1.017	7.451
		C	35.76	83.89	38.55	1.946	5.471	29.17	1.018	6.404
8	$P2_12_12_1$	A	12.53	23.74	7.08	0.909	1.451	5.17	0.718	1.843
		E	12.39	23.85	7.45	0.890	1.534	5.66	0.701	1.891
		C	24.90	51.17	18.15	1.488	2.728	10.88	0.939	3.533
9	$P2_12_12_1$	A	14.86	29.80	10.28	0.980	1.840	7.58	0.733	2.251
		E	18.90	41.37	17.13	1.100	2.701	13.27	0.740	3.123
		C	39.88	91.47	40.39	1.935	4.914	24.77	1.034	5.942

Kiefer & Wilson, 1985) and this aspect is beyond the scope of the present paper.

The authors are grateful to Dr M. N. Ponnuswamy and co-workers and Dr D. Velmurugan for providing CAD-4 diffractometer intensity data for some of the crystal structures used in testing the theoretical results. They also thank the referees for useful comments. Thanks are due to the Council of Scientific and Industrial Research, India, for the award of a Senior Research Fellowship to KS.

References

ABRAMOWITZ, M. & STEGUN, I. A. (1965). *Handbook of Mathematical Functions.* New York: Dover.

EADIE, W. T., DRIJARD, D., JAMES, F. E., ROOS, M. & SAADOULET, B. (1972). *Statistical Methods in Experimental Physics.* Amsterdam, London: North-Holland.

FOSTER, F. & HARGREAVES, A. (1963). *Acta Cryst.* **16**, 1133-1139.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

PARTHASARATHY, S., PONNUSWAMY, M. N., ELANGO, N. & SEKAR, K. (1990). *Acta Cryst.* **A46**, C37.

PONNUSWAMY, M. N. & KANDASAMY, M. (1990). Personal communication.

SEKAR, K. (1991). PhD thesis, Univ. of Madras, India.

SEKAR, K., PARTHASARATHY, S., EPP, B. & MONDON, A. (1992). Personal communication.

SEKAR, K., PARTHASARATHY, S., PRABAHAR, K. J. & RAMAKRISHNAN, V. T. (1993). *Acta Cryst.* **C49**. In the press.

SEKAR, K., PARTHASARATHY, S. & RADHAKRISHNAN, T. R. (1993). *Acta Cryst.* **C49**. In the press.

SEKAR, K., PARTHASARATHY, S. & RAJALINGAM, P. (1990). *Acta Cryst.* **C46**, 1153-1155.

SHANMUGASUNDARRAJ, S., PONNUSWAMY, M. N., SHANMUGAM, G. & KANDASAMY, M. (1992). Personal communication.

SHMUELI, U., WEISS, G. H. & KIEFER, J. E. (1985). *Acta Cryst.* **A41**, 55-59.

SRINIVASAN, R. & PARTHASARATHY, S. (1976). *Some Statistical Applications in X-ray Crystallography.* New York: Pergamon.

SRINIVASAN, R. & SUBRAMANIAN, E. (1964). *Acta Cryst.* **17**, 67-68.

VELMURUGAN, D. (1991). Personal communication.

VELMURUGAN, D. (1992). Personal communication.

WEISS, G. H., SHMUELI, U., KIEFER, J. E. & WILSON, A. J. C. (1985). *Structure and Statistics in Crystallography,* edited by A. J. C. WILSON, pp. 23-42. New York: Adenine Press.

WILSON, A. J. C. (1949). *Acta Cryst.* **2**, 318-321.