SHORT COMMUNICATIONS

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Statistical analysis of structure-factor residuals.

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Structure-factor residuals have been analysed statistically for deviation from a normal distribution. The moments of skewness and kurtosis indicate whether the data are free from systematic error.

In order to determine the precision of a crystallographic determination it is customary to use the residual index (Stout & Jensen, 1968). We have analysed the structure-factor residuals statistically for deviation from a normal distribution. This indicates if the data are free from systematic error, and subject solely to random error.

Table 1. *Statistical analysis of structure-factor residuals* [*data from Shields & Kennard* (1977)]

Structure	R	$\bar{\Delta}$	σ	α_3	α_4	$0{\cdot}7979\sigma$	$\bar{\sigma}$	Number of observed reflexions	Number of unobserved reflexions
1,1-Bis(*p*-chlorophenyl)acetic acid (DDA)	0·091	0·741	1·745	0·732	4·715	1·392	1·310	1600	1321
1,1-Dichloro-2,2-bis(*p*-chlorophenyl)-ethane (DDD)	0·068	0·351	1·681	0·567	4·635	1·341	1·249	877	456
1,1-Dichloro-2,2-bis(*p*-chlorophenyl)-ethylene (DDE)	0·049	0·173	0·996	0·611	6·105	0·795	0·707	1751	856
4,4′-Dichlorobenzophenone (DBP)	0·088	0·865	3·324	0·462	4·399	2·653	2·501	726	314
Ideal (normal distribution)		0		0	3·0				

If we have a sample of N values of the residual Δ, then in a complete universe, the arithmetic mean, μ, should be 0, and an experimental arithmetic mean $\bar{\Delta}$ close to 0. At the same time, the moment coefficient of skewness (α_3) and kurtosis (α_4) may also be calculated. For a normal distribution, $\alpha_3 = 0$, $\alpha_4 = 3$ and the mean deviation $= \sigma\sqrt{(2/\pi)} = 0{\cdot}7979\sigma$.

The last result may be compared to a calculated mean deviation $\bar{\sigma}$. These statistical terms are defined in Spiegel (1961), and other books on statistics. So far a number of refined structures have been tested and they all show a considerable degree of skewness and kurtosis (Table 1). No doubt there are many unaccounted for errors due to model, scale, use of spherical scattering factors, elliptical temperature factors, extinction, absorption, *etc.* These have been discussed by Abrahams & Keve (1971).

References

ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* A27, 157–165.

SHIELDS, K. G. & KENNARD, C. H. L. (1977). *J. Chem. Soc. Perkin* II, pp. 460–463.

SPIEGEL, M. R. (1961). *Theory and Problems of Statistics.* New York: Schaun.

STOUT, G. H. & JENSEN, L. H. (1968). *X-ray Structure Determination*, p. 245. New York: Macmillan.