Some comments on the papers S. (1974), S. & V. (1975) and S. (1975) are given in the Appendix.*

Note added in proof: The most recently published results on the doubling of the *c* axis in monoclinic WO_3 (Lefkowitz, Dowell & Shieldt, 1975) confirm the equivalence of the lattice directions in WO_2Cl_2, monoclinic WO_3 and orthorhombic WO_3 given here, as well as earlier results (Schröder & Felser, 1972).

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* The Appendix has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31508 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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The residual in the case of a mixture of centric and acentric reflexions.

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The value of the residual for a randomly wrong structure when calculated from a mixture of centrosymmetrical and non-centrosymmetrical structure factors is close to the value obtained by interpolation between the centric and acentric cases of Wilson [*Acta Cryst.* (1950). **3**, 397–398].

Wilson (1950) pointed out that it was useful to know the likely value of the crystallographic residual for a randomly wrong structure, and he showed that this was $2\sqrt{2}-2$ if the Wilson (1949) centric distribution function applies, and $2-\sqrt{2}$ if his acentric distribution function applies. In non-centrosymmetrical space groups other than $P1$, one has both centrosymmetrical and non-centrosymmetrical structure factors, and usually calculates the residual without separation of the structure factors into two sets.

From equations (1) and (5) of Wilson's 1950 paper

$$R_{\text{random}}=\frac{2\langle F\rangle-4\langle G(F)\rangle}{\langle F\rangle}$$

where

$$G(F)=\int_0^F F'P(F')\mathrm{d}F'.$$

If a proportion c of the structure factors belongs to the centric distribution, and $(1-c)$ to the acentric,

$$R_{\text{random}}=\frac{2c\langle F\rangle_C+2(1-c)\langle F\rangle_A-4c\langle G\rangle_C-4(1-c)\langle G\rangle_A}{c\langle F\rangle_C+(1-c)\langle F\rangle_A} \quad (1)$$

where the subscripts C and A refer to the centric and acentric distributions used to average F and G. Values of these averages are given by Wilson (1950): substitution in (1) gives

$$R_{\text{random}}=\frac{(4-2\sqrt{2})c+\pi(1-\sqrt{2}/2)\,(1-c)}{\sqrt{2}c+\dfrac{\pi}{2}(1-c)} \quad (2)$$

which reduces to Wilson's equations (8) and (10) when $c=1$ and 0 respectively. A straight line interpolation between the limiting values is given by

$$R_{\text{random}}\approx 2-\sqrt{2}+(3\sqrt{2}-4)c$$
$$\approx 0.59+0.24c\,. \quad (3)$$

Use of (3) rather than the more exact (2) involves an error never greater than 0.006.

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