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## Absorption corrections for neutron diffraction.

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**Abstract**

The transmission factors tabulated by Rouse, Cooper, York & Chakera [*Acta Cryst.* (1970), A**26**, 682–691] for $\mu r < 1$ can be expressed as the product of two factors: a scale factor and a Debye–Waller factor. In the case of a sphere or a cylinder, the absorption corrections then reduce to simple adjustments of these parameters at the end of the refinement, instead of tedious corrections to the data itself. The results are of particular use for powder data. A printing error in the original paper is also corrected.

Absorption corrections are usually made by reference to a tabulation of the transmission factor $A_{hkl}$, or by the use of computer programs to correct the raw data. For example, Rouse, Cooper, York & Chakera (1970) have produced a table particularly suited to neutron diffraction, where usually $\mu r < 1$. Of course the use of such tables is tedious, and when computer programs are available it is not always clear what the effect will be of errors in the measurement of the absorption coefficient $\mu$, the crystal radius $r$, or even the different approximations used to calculate $A_{hkl}$.

Rouse *et al.* also give an analytical approximation for $A_{hkl}$, where the error does not exceed 0·0035 for $\mu r < 1$ ($1 > A_{hkl} > 0{\cdot}1965$):

$$A_{hkl} = \exp[-(a_1 + b_1 \sin^2\theta)\mu r - (a_2 + b_2 \sin^2\theta)(\mu r)^2],$$

where the coefficients are:

| | Cylinder | Sphere |
|---|---|---|
| $a_1$ | 1·7133 | 1·5108 |
| $b_1$ | −0·0368 | −0·0315 |
| $a_2$ | −0·0927 | −0·0951 |
| $b_2$ | −0·3750 | −0·2898. |

(Note that there is a printing error for $b_2$ in the original paper.) Clearly this expression can be rewritten as

$$A_{hkl} = k \exp[-\Delta B (\sin\theta/\lambda)^2],$$
$$k = \exp[-a_1\mu r + a_2(\mu r)^2],$$
$$\Delta B = \lambda^2[b_1\mu r + b_2(\mu r)^2],$$

where $k$ is a scale factor and $\Delta B$ is an overall Debye–Waller factor.

Then, unless absolute measurements are being made, the absorption correction for spherical or cylindrical samples can be performed at the end of the refinement simply by adding $\Delta B \cos\gamma^*$ to all the $B_{ij}$, where $\gamma^*$ is the angle between the reciprocal-lattice axes $i$ and $j$.

The result is of particular use for neutron powder diffraction where the product $\mu r$ can be obtained simply by measuring the transmission through a fine slit placed in front of the sample. For example, a value of $\mu r = 0{\cdot}579$ was obtained for a 16 mm diameter sample of $CsPbCl_3$, giving $\Delta B = 0{\cdot}27$. Even for a weakly absorbing sample of deuteronaphthalene, we found $\mu r = 0{\cdot}274$ and hence $\Delta B = 0{\cdot}07$. In most cases, absorption corrections are not made for neutron powder diffraction, and this results in significant underestimations of the Debye–Waller factors, even for apparently weakly absorbing materials. Given the ease with which the above formulae can be applied, there is now no excuse for not making these corrections.

The concurrence of M. J. Cooper with these comments on his original paper is acknowledged.

**Reference**

ROUSE, K. D., COOPER, M. J., YORK, E. J. & CHAKERA, A. (1970). *Acta Cryst.* A**26**, 682–691.

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## Errors in coordinates, bond lengths, and bond angles.

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**Abstract**

Standard deviations in bond lengths and bond angles are related to standard deviations in atomic coordinates according to published equations [Cruickshank (1959). *International Tables for X-ray Crystallography*. Vol. II, pp. 331–332]. These equations were derived for an idealized model in which the distribution of coordinate errors is isotropic. Tests show that typical structures exhibit only moderate deviations from this model, and so the calculated standard deviations are accurate. Furthermore, the standard deviation in a bond angle $\varphi$ (in degrees) can be well approximated by the expression $\sigma(\varphi) \sim 81\ [\sigma(R)/R]_{\text{r.m.s.}}$, where the quantity in square brackets is the root-mean-square value of $\sigma(R)/R$ for

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