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Determination of the degree of crystallinity of polyphenylene sulfide composited with crystalline and non-crystalline fillers by applying the direct derivation method. Corrigendum

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An erroneous equation and some values of related parameters in the paper by Toraya [J. Appl. Cryst. (2024), 57, 1115–1126] are corrected.

In the paper by Toraya (2024), the first equation in equations (17) on page 1118 was erroneously given. The disorder factor D, defined by $D = \exp[-d(2\sin\theta/\lambda)^2]$, should not be a multiplier but a divider. The correct equation is given by

$$Y_{P_C}^{T_n}(d) = \int_{2\theta_{L}}^{2\theta_{T_n}} y(2\theta)_{P_C}^{obs} \left\{ \exp\left[-d\left(\frac{2\sin\theta}{\lambda}\right)^{2}\right] \right\}^{-1} G(2\theta) \, \mathrm{d}(2\theta).$$

Since $\left[\exp(-dx^2)\right]^{-1} = \exp(dx^2)$ and d is optimized together with the degree of crystallinity, D_0 , during the minimization of the cost function S [equation (18)], the influences on the derived D_0 values were considered to be small. The D_0 and d parameters were recalculated with the correct equation, and they are given in Table 1. The differences in d values between the two calculations were, in this case, very small. Actually, the individual $\overline{D_0}$ values were almost unchanged, and their differences from the previous ones were within $\pm 0.1\%$.

References

Toraya, H. (2024). J. Appl. Cryst. 57, 1115-1126.

