

MS45-O3 Empirical correction for resolution- and temperature-dependent errors caused by factors such as thermal diffuse scattering

Keywords: data quality, thermal diffuse scattering

Regine Herbst-Irmer¹, Benedikt Niepötter¹, Dietmar Stalke¹

1. Institute of Inorganic Chemistry, Georg-August-University Göttingen

email: rherbst@shelx.uni-ac.gwdg.de

Charge density investigations of several compounds conducted at multiple temperatures show two disturbing features. First, the models derived from these high resolution datasets at different temperatures differ significantly. Additionally, residual density appears close to or even at the atomic positions, especially for datasets measured at 100 K. This indicates significant errors that could be caused by thermal diffuse scattering (TDS).

TDS mainly results in an underestimation of the atomic displacement parameters. However, smaller but nevertheless important errors occur in other parameters as well [1]. Hence the heights of the maxima in the electron density are changed at the same location [2, 3]. First order TDS leads to peak broadening in the diffraction experiment.

A reduction of the integration box size leads to a substantial improvement in quality and diversity of the models. At the same time it indicates TDS to cause these errors. However, this method is very time-consuming and an alternative is needed.

It is possible to estimate the TDS contribution by analyzing the peak profile [4]. Extending this idea programs were developed to assess the TDS contribution to the measured intensities for data collected with point detectors [5, 6].

In endeavouring to improve the method, it was noticed that the refinement of resolution-dependent scale factors can be employed as a validation tool to detect such errors. In a nested interval approach a correction factor [7] is determined that minimizes these errors and improves the model quality [8].

[1] Alexandropoulos, N. G., Cooper, M. J., Suortti, P. & Willis, B. T. M. (2006). *International Tables for Crystallography*, Vol. C, edited by E. Prince, pp. 653–665, 1st online ed. Chester: International Union of Crystallography.

[2] Tsirelson, V. G. & Ozerov, R. P. (1996). *Electron Density and Bonding in Crystals: Principles, Theory and X-ray Diffraction Experiments in Solid State Physics and Chemistry*. Bristol, Philadelphia: Institute of Physics Publishing.

[3] Helmholdt, R. B. & Vos, A. (1977). *Acta Cryst.* **A33**, 38–45.

[4] Jennings, L. D. (1970). *Acta Cryst.* **A26**, 613–622.

[5] Blessing, R. H. (1987). *Crystallogr. Rev.* **1**, 3–58.

[6] Stash, A. & Zavodnik, V. (1995). *Crystallogr. Rep.* **41**, 404–412.

[7] Zavodnik, V., Stash, A., Tsirelson, V., de Vries, R. & Feil, D. (1999). *Acta Cryst.* **B55**, 45–54.

[8] Niepötter, B., Herbst-Irmer, R. & Stalke, D. (2015). *J. Appl. Cryst.*, **48**, 1485–1497.