An Empirical Correction for Thermal Diffuse Scattering?

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Thermal diffuse scattering (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 without displacing them. [2,3] First order TDS leads to peak broadening in the diffraction experiment. As shown by Jennings [4] it is possible to estimate the TDS contribution by analyzing the peak profile. Blessing [5] as well as Stash and Zavodnik [6] extended this idea and developed programs to assess the TDS contribution to the measured intensities for data collected with point detectors. However, with area detectors these methods were no longer useable. Currently the effects of TDS on the model are more or less ignored referring to the low temperatures during the measurement. Nevertheless problems due to TDS can occur also at 100 K or even at 15 K. Residual density appears close to atomic positions. Therefore it is essential for high quality single crystal X-ray experiments to correct for TDS.
By refining resolution dependent scale factors it is possible to minimize the residual density. In a simple approach the known ideas [7] are transferred to area detector techniques. By iteratively determining the correct size of the integration box the influence of TDS is minimized. An empirical TDS correction for the measured intensities can be derived from these methods. Model improvements will be demonstrated.

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