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MS20 Rating and improving data quality: instrumentation, analysis and postprocessing

Chairs: Dr. Karine Röwer, Dr. Loes Kroon-Batenburg

MS20-O1

Experimental charge density studies: improvements in data processing

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In experimental charge density investigation, it is indispensable to use the highest possible quality of data. Systematic errors should be avoided.

One systematic error is the low-energy contamination caused by focusing multilayer optics. To eliminate this problem filtering by interposition of a low-density material foil into the beam was proposed. However, filtering lowers the intensity, which might be crucial, especially for charge density data collection, and is of course not possible for already measured data. The low-energy contamination mainly affects the reflections with indices 3h 3k 3l. In the program SADABS [1], a 3λ correction in analogy to the earlier 2/λ correction is now implemented. [2]

In several charge density studies, we noticed that the residual density improved significantly after ten resolution dependent scale factors were refined. The dependency of the scale factors against resolution showed a typical pattern for all data sets, but the variation was much smaller for data collected at 15 K instead of 100 K. Therefore, this procedure seems to cure errors that are resolution and temperature dependent such as thermal diffuse scattering (TDS). Similar results could be obtained by processing data with relatively small integration boxes instead of refined box sizes. This procedure seems to emulate a rough TDS correction. However, to find the best integration box is very time consuming. In a nested interval approach, a correction factor $\{\alpha = a[\sin(\vartheta)/\lambda]^2 + b[\sin(\vartheta)/\lambda]^3\}$ is determined that minimizes these errors and improves the model quality. [3]

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