MS38-P04 | MEASURING ACCURATE SINGLE CRYSTAL DIFFRACTION DATA USING A PILATUS3 CDTE DETECTOR

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Pilatus3 detectors were released in 2012 and are widely established in macromolecular crystallography with over 4,000 PDB entries. The specifications of the Pilatus3 CdTe were quickly recognized as promising in charge density investigations, mainly due to the detection efficiency in the high-energy X-ray regime. Moreover, the dynamic range and low noise should overcome the perpetual problem of detecting strong and weak data simultaneously. However, to the best of our knowledge there is no publication available presenting high resolution data collected with a Pilatus3 CdTe detector.

Our experience with this detector family revealed two aspects that lead to systematically underestimated intensities at the two extremes of the detected intensity scale. Herein, Rubrene and $FeSb_2$ are representatives for the two cases. Additionally, a LaB_6 powder sample was consulted to validate the findings of the single crystal studies where counting statistics and reproducibility are more delicate.

The first aspect is indicated by systematically too low intensities for weak reflections, revealed by a variation of exposure time and beam attenuation. The origin was found in the data processing, specifically in the outlier rejection and data averaging.

The second case affects the most intense reflections and is connected to the maximum flux of the diffracted beam but not the total number of counts. We utilized a maximum flux estimation procedure to identify unproblematic flux ranges. Disregarding this issue leads to unreasonably large extinction parameters.

Our results conclude that only the combination of careful data collection and processing can result in high quality data.