

MS39-P3 CrysAlisPro 38: Data quality, fast experimentation, AutoChem 2.1 & StructureExplorer

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Data quality critically relies on proper instrument calibration. Our new version 38 of CrysAlisPro features a new approach to calibration enhancing the instrument description and thus giving better data quality. Improved hardware and software allow high speed data acquisition. Multi-threaded acquisition and reduction pipelines allow fast concurrent data reduction. The 'What is this?' tool gives chemical connectivity information in less than 1min. AutoChem 2.1 offers a fine tuned structure completion algorithm and integrates the latest structure solution and refinement tools. It also offers a new structure visualizer called 'StructureExplorer'. It tightly links with the AutoChem 2.1, the external Olex2 program and internal data processing offering the user an easy handling of the structure from solution to report.

Keywords: Data processing, area detectors, automation

MS39-P4 Powder diffraction in Bragg-Brentano geometry with straight linear detectors

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Powder diffraction as one of the most common material characterization tools is significantly benefiting from the recent developments in detector technology. One and two-dimensional detectors are nowadays commonly used to speed up the acquisition of powder diffraction data. This usually goes hand in hand with worse resolution and asymmetric peak profiles [1, 2]. In our presentation the influence of a straight linear detector on the resolution function in the Bragg-Brentano focusing geometry is discussed [3]. Because of the straight nature of most modern detectors geometrical defocusing occurs, which heavily influences the line shape of diffraction lines at low angles. To circumvent this problem we suggest an easy approach in which an adaptive range of channels of the linear detector is used at low angles. This results in an improved resolution especially at low angles. At higher angles the whole linear detector is used and the data collection remains fast. Using this algorithm a well behaved resolution function is obtained in the full angular range, whereas simply using the full linear detector the resolution function varies within one pattern, which hinders line-shape and Rietveld analysis.

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