ACCURATE EXPERIMENTAL CHARGE DENSITY DATA: TIPS & TRICKS FOR DATA COLLECTION & PROCESSING

Holger Ott, Bruker AXS GmbH, e-mail: holger.ott@bruker.com

A number of recent hardware developments enable scientists working in Quantum Crystallography to collect best ever crystallographic data in shorter time and with greatest convenience.[1] High-brilliance sources, such as the first generation of IµS DIAMOND microfocus sources (Mo K\textsubscript{α} and Ag K\textsubscript{α}) and the METALJET (In K\textsubscript{α}) go along with large active area, mixed-mode photon counting pixel array detectors (PAD) for highest system efficiency.

Despite all advances in automation for strategy planning and data processing, the careful selection of a good crystal and the thorough execution of the experiment are still of crucial importance. For best results in this advanced crystallographic field the experimentalist ideally has a certain level of experience and carefully follows to the rules of Good Crystallography Practice (GCP).

This presentation will provide proven tips & tricks to make the charge density research more successful. This includes suggestions to optimize the instrument performance, but also GCP aspects. The presentation will also highlight recent improvements of the APEX3 software suite with a focus on special options particularly important to the field.[2]

References
