It's all about the numbers: Achieving best-quality data with the Bruker PHOTON III CPAD detector

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The single overarching requirement for a high-quality structure determination is excellent counting statistics. High quality data is defined by the overall resolution limit, the accuracy of the measured reflection intensities, and the signal-to-noise ratio. These requirements can be met only by careful measurement of the data set. Running at cross purposes in modern laboratories is the pressure to push experiments through the queue. Compounding this, many smaller, weakly diffracting specimens require longer wavelength X-ray sources like copper sources, which necessitate observation of larger volumes of reciprocal space to achieve adequate resolution. Charge density studies are performed to the highest resolution possible, as high as 0.36 Å for molybdenum radiation. Consequently, there is a need to measure both weak signals and strong signals simultaneously and efficiently, especially through these larger volumes. The Bruker PHOTON III family of detectors excels here. The PHOTON III is capable of single-photon counting and simultaneous signal integration with a range of source energies, eliminating noise and maximizing signal quality. With large-format sensors, as large as 20 x 14 cm^2, the PHOTON III also quickly covers the large volumes required for high-resolution data sets. The practical impacts for the laboratory will be explored in this presentation through the examination of a series of small-molecule samples that illustrate the range of problems that are commonly encountered in real samples. Small, weakly diffracting crystals of light-atom chiral compounds have been studied, as have mineralogical samples and coordination compounds. Details of these experiments will be highlighted.