MS20-P12

A photon-counting, large-area detector – PHOTON III

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The appearance of significantly stronger third generation synchrotron sources at large scale facilities and microfocus technology using in-house sources has led to the replacement of imaging plates by CCD, CMOS and HPAD detectors. Current state-of-the-art HPAD detectors, such the PHOTON II, deliver impressive results and have allowed the collection of the first in-house GPCR structure only a few months ago.

Modern synchrotron beamlines show a preference for largest possible detectors, which provide a number of advantages:

- Increased sample-detector distance results in reduced background X-ray scattering with improved signal-to-noise measured from weakly diffracting samples
- More reflections are collected per frame, reducing the radiation dose and overall measurement time
- Efficient collection of complete data at high resolution
- Better signal separation from reflections of very long unit cell axes

The Detective Collection Efficiency (DCE) is an established measure to describe the productivity of an X-ray detector[1]:with Ω being related to the active area size, DQE to the sensitivity of the detector and t_{read} to the read out dead time unit. The new PHOTON III is a detector for structural biology, which improves the DCE from two ends:

- The detector has a large active area of 280 cm^2, resulting in a DCE two-times greater than the PHOTON II
- The detector is operated in a newly developed photon counting mode.

The PHOTON III offers large active-area detectors to the home laboratory at affordable costs. Like all our CPAD detectors the PHOTON III has zero read out time, does not suffer from charge charging effects and satisfies the Shannon-Nyquist theorem. Even better, this goes along with a remarkable improvement in background suppression using the newly developed photon counting mode.

Apart from a discussion of technical details the presentation will focus on first data sets collected with the new detector.

$$DCE = \frac{\Omega}{4\pi} DQE \left(1 + {}^{t_{read}}/_{t_{frame}}\right)^{-1}$$

References:

[1] Stanton M (1993) Nuc. Instrum. and Meth. in Phys. Res. A 325(3),550-557.

MS20-P13

Highest Data Quality with Latest In-House Sources and Detector Technology

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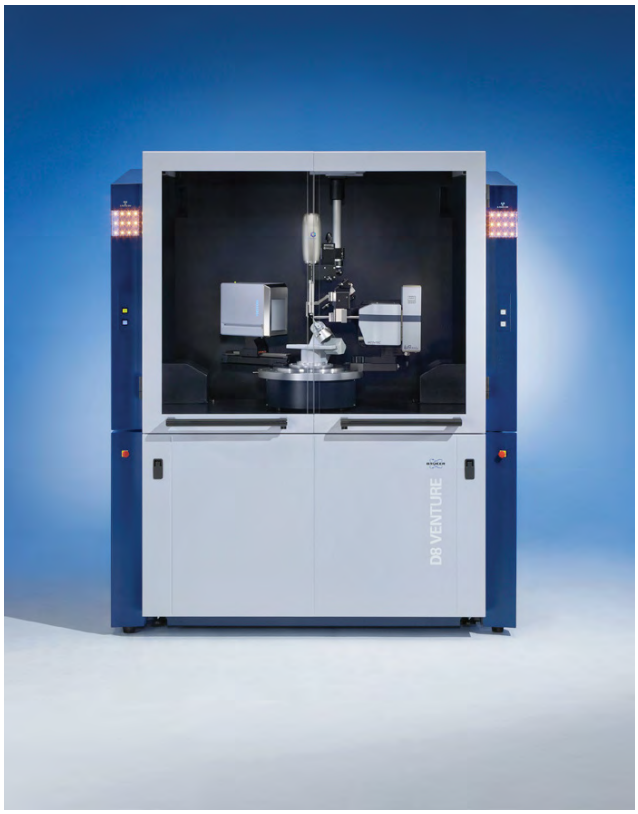
Modern chemical and biological crystallography continuously pushes the limits to ever smaller samples with typically weaker diffraction properties. Here we will present a number of structures obtained from extremely challenging samples. Experimental data collected on an in-house system illustrate the strength of two new components which tremendously improve the performance of laboratory instrumentation: the new ImS DIAMOND source and the new PHOTON III X-ray detector.

The air-cooled ImS DIAMOND microfocus sealed tube source uses a unique diamond hybrid anode technology to produce intensities similar to modern microfocus rotating anodes. The anode consists of a diamond substrate coated with copper. The high thermal conductivity, low thermal expansion and extreme hardness of diamond make it an ideal substrate, which allow for higher power loading and greater long-term stability of the source, delivering the brightest micro-focus sealed tube ever.

As of today another problem associated with high-end X-ray sources is gone: high maintenance costs. The ImS DIAMOND does not require any routine maintenance and has the same legendary life time which makes the ImS system the most popular microfocus X-ray source for more than a decade.

The PHOTON III is a new CPAD (charge-integrating pixel array detector), which utilizes a mixed-mode approach for data collection. The weak reflections are measured in photon-counting mode and the strong reflections are measured in integrating mode. Consequently, the ultra-sensitive PHOTON III detector can collect very weak reflections without suffering from charge-sharing or non-linearity effects common to other photon-counting detectors.

Bruker's D8 QUEST and D8 VENTURE both take advantage of these improvements in source and detector technology, leading to a previously unknown level of performance without increasing operational costs.



MS21- Intermolecular interactions from structural, energetic and charge density perspective(s)

Chairs: Prof. Enrique Espinosa, Prof. Ulli Englert

MS21-P01

Crystal structure and reconstruction of charge density of 9-aminoacridine hemihydrate

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Nowadays, the most routine X-ray structure determination in crystallography is based on so-called Independent Atom Model (IAM) of electron density, which assumes both sphericity and neutrality of the atoms. Unfortunately, the quantitative topological analysis of an electron density based on IAM is inaccessible (Dittrich *et al.*, 2009). The multipolar approach, as proposed by Hansen and Coppens (Coppens, 1997) , is the method of choice in modelling of the experimental electron density distribution. High-resolution diffraction data of outstanding quality are mandatory in order to perform full structure refinement with multipolar model – a condition impossible to meet for very small crystals or macromolecules. However, the theoretical databanks of aspherical scattering factors developed in recent years, for example, UBDB databank (Jarzembska & Dominiak, 2012) based on experimental geometries, can be used in order to reconstruct the charge density with the Transferable Aspherical Atom Model (TAAM) approach.

Acridines belong to the polycyclic heteroaromatic chemical compounds and their derivatives have found a wide range of applications in clinical area as an antimicrobial, antiviral or antitumor agents as well as in chemical analysis, for example as a matrix for matrix-assisted laser desorption/ionization (MALDI). The 9-aminoacridine can be considered as a model compound from this family of chemicals. In its neutral form it crystallizes as a hemihydrate the $I\,4_1/a\,2/c\,2/d$ space group with several atoms in special positions. The very interesting crystal structure of title compound was described in the 1983 year by Chaudhuri and until now has not been more thoroughly investigated. Here, the reconstruction of charge density distribution with the UBDB data bank and TAAM refinement will be performed in order to obtain more accurate geometry of the compound, the quantitative topological analysis of an electron density as well as the basis for the energetic calculation (crystal lattice and dimer energies) by using *Crystal*, *CrystalExplorer* or *Pixel* approaches. This research is the part of the wider project carried out in cooperation with dr Mihails Arhangelskis.