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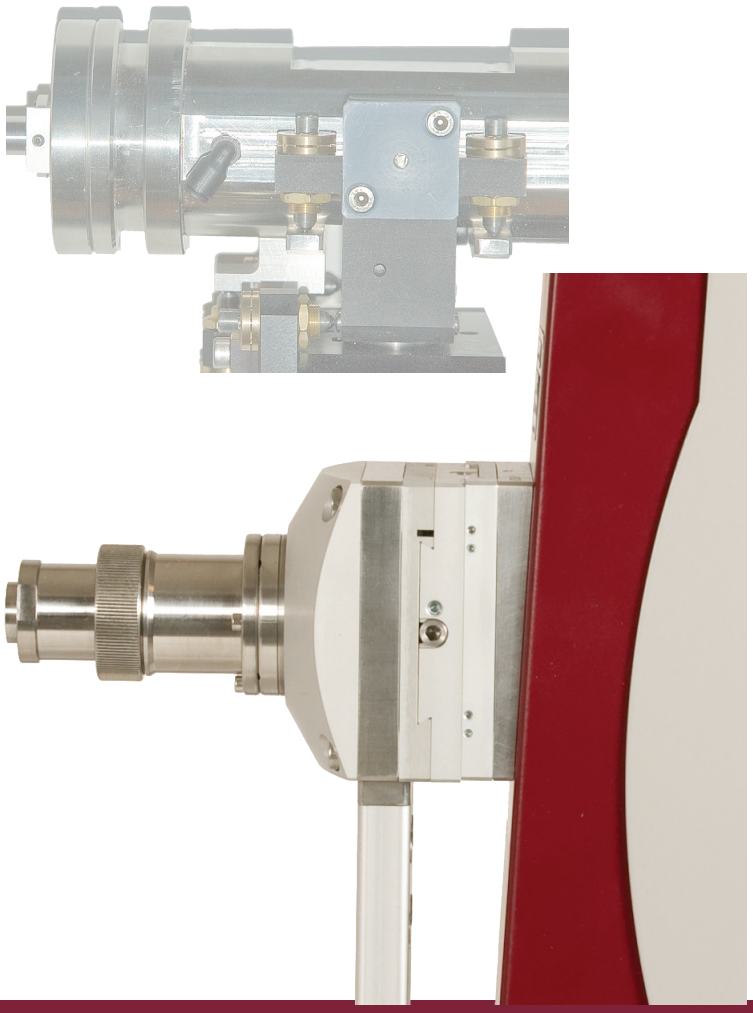

Comparison of the GeniX 3D Cu HF beam delivery system with the GeniX Cu VHF system

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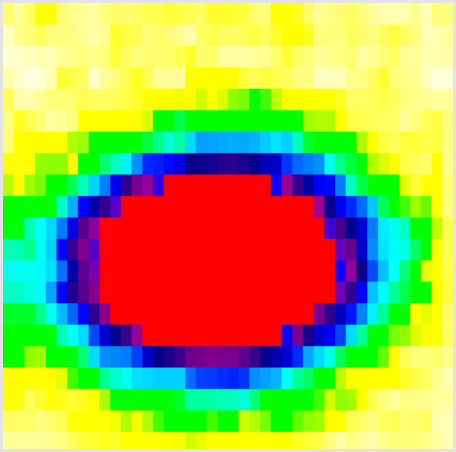
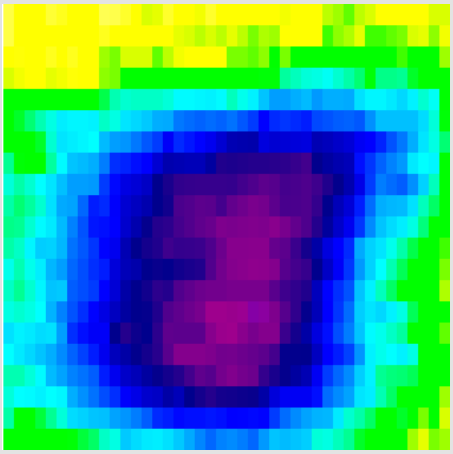
Introduction

The marμX system is a very compact yet powerful complete X-ray setup suitable for both protein and small molecule data collection as well as other types of experiments. The marμX system consists of a mar345 image plate detector, a mardtb goniometer system and the new 2010 model of the GeniX 3D Cu HF generator operated at 30 W (50 kV / 0.6 mA).

In this study we compare the new GeniX 3D Cu HF system with the previous GeniX Cu VHF generator operated at 50 W (50 kV / 1.0 mA). The new system features an entirely new tube setup including a newly designed and highly optimized X-ray optic. Thanks to a number of major improvements the new generator delivers more X-ray photons onto the sample despite of running at lower power (30 W instead of 50W).

In order to asses the quality of the new system, several small molecules of different types and sizes have been collected. Here we present a selection of typical results.

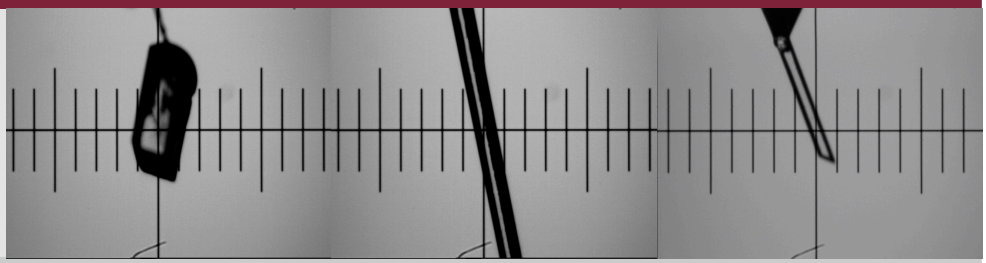
Technical Data

	New GeniX	Old GeniX
Beam at crystal position The picture show an area of **0.5 x 0.5**. The color coding reflects the measured intensity of the beam.		
Distance source - optic center	8 cm	14 cm
Distance optic center - focus	30 cm	39 cm
Spot size in focus	175 µm x 175 µm	190 µm x 190 µm
Flux within 100 µm at focus	9 x 10^7 photons/sec	5 x 10^7 photons/sec
Divergence (mrad @ FWHM)	~ 6 x 6	5.4 x 5.4

Data collection and processing

The data for all crystals were collected on the same mar345dtb detector system. When exchanging the generators, the beam was carefully realigned. The crystals needed to be taken off the goniometer but they were remounted in a position very close to where they have been mounted before. Data were collected at:
- 90 mm distance crystal-to-detector giving 1.5 Ang. resolution at the edge
- 5 deg./image
- 72 images (i.e. 360 deg. of data)
- constant exposure time (typically 40s/image)

Data were processed using the automar program suite.

	Anil		Bitartrate1		Bitartrate2	
Crystal						
Space group	P 1		$P\,2_12_12_1$		$P\,2_12_12_1$	
Unit cell axes a, b, c	a=9.7 b=13.5 c=16.7		a=7.6 b=7.8 c=11.1		a=7.6 b=7.8 c=11.1	
Mosaicity	0.6^0		0.6^0		0.3^0	
Size of crystal W x H x L	350 x 180 x 500		120 x 120 x 2000		30 x 60 x 500	
Optics	**NEW**	**Old**	**NEW**	**Old**	**NEW**	**Old**
# reflections	4166	4194	1287	1316	1417	1387
Multiplicity	3.5	3.6	9.8	9.9	10.5	10.3
Rsym	4.4	4.5	3.6	3.7	3.1	3.6
<Intensity>	12276	8717	100706	57667	29244	23734
Scale $\langle I\rangle_{NEW} : \langle I\rangle_{Old}$	**1.41**		**1.75**		**1.23**	

Conclusion

The net intensities of reflections in the final data set depend on several factors:
- the amount of X-rays photons delivered by the generator in a small area
- divergence of X-ray beam
- size of crystal
- mosaicity of crystal

It is very difficult if not impossible to crystallographically separate the contributions of those individual factors. Still, by comparing the diffracted net intensities of a number of crystals of different sizes and forms, meaningful conclusions can be drawn about the performance of the X-ray equipment. In this study, we conclude that within limits of accuracy, the new Genix 3D Cu HF source is stronger than the previous model despite of running at lower power. The gain in performance for crystallographic purposes is in the same order of magnitude as the specified X-ray photon flux, up to 1.8.