X-ray diffractometer system with single or dual PhotonJet microfocus sources

XtaLAB Synergy

1. Introduction

With your success utmost in our minds, the XtaLAB Synergy has been developed for single crystal X-ray diffraction. Using a combination of leading edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy produces **fast**, **precise** data in an **intelligent** fashion.

2. Features

2.1. Goniometer

An improved κ goniometer design provides greater access to reciprocal space and both longer and shorter crystal to detector distances. Motor speeds have been doubled to improve data collection speed and minimize dead-time between scans. Total data acquisition time has been reduced and the ability to analyze smaller samples is improved by newly designed PhotonJet™ X-ray sources.

Table 1. PhotonJet options for the XtaLAB Synergy.

Target	Power/Voltage	Increase in fluence (ph/sec/mm^2)
Cu	50 W/50 kV	>100%
Mo	50 W/50 kV	>75%
Ag	44 W/65 kV	>100%

2.2. X-ray source

The XtaLAB Synergy can be equipped with either one or two PhotonJet X-ray sources (Fig. 1) from a selection of three radiation types: Cu, Mo, and Ag (Table 1). The PhotonJet X-ray source is based on microfocus sealed-tube technology and includes a new X-ray tube, new optics, and new alignment mechanism providing double the fluence and longer tube life compared to previous sources.

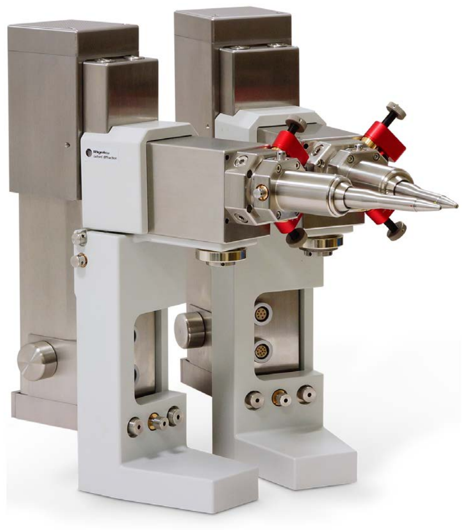

Fig. 1. New PhotonJet X-ray source incorporate new X-ray tubes, new optics and improved alignment mechanism.

2.3. Detectors

The new HyPix-6000HE detector (Fig. 2), a next-generation two-dimensional semiconductor detector designed specifically to meet the needs of the home lab diffractionist. The HyPix-6000HE is a Hybrid Photon Counting (HPC) detector with a large active area of approximately 6000 mm^2, a small pixel size of 100 μm^2, a high count rate of greater than 10^6 cps/pixel, with the ability to measure data in a true shutterless mode.

Fig. 2. New HyPix-6000HE detector.

Each pixel on the HyPix-6000HE detector has dual energy discriminators, which makes it possible to adjust the energy window width by setting the energy threshold to "high" and "low," respectively. The low-energy discriminator can eliminate electrical noise and reduce fluorescence background, and the high-energy discriminator can eliminate cosmic rays and white radiation. As a result, data can be measured with an optimized signal-to-noise ratio.

The XtaLAB Synergy may also be equipped with the Eos S2 or Atlas S2 CCD detectors. These modern detectors are fast and sensitive over a wide range of X-ray energies and are well suited for Ag radiation. They have also the ability to measure data with very high dynamic range thanks to the instant binning control and software-controlled self-optimizing sensitivity.

2.4. Cabinet

A new user-inspired cabinet design includes additional space for an improved work environment and electronically controlled brightness of the cabinet interior and crystal lighting, which results in optimum video imaging for all types of crystal samples.

Safety is an important concern, particularly in multi-user environments. The XtaLAB Synergy has an entirely new dedicated safety module that is designed to protect you and to meet the highest possible safety standards in the world.

2.5. Software

The highly regarded CrysAlis^{Pro} software package is the nerve center of the XtaLAB Synergy, tying together all the new improvements of speed and fluence through a highly parallelized architecture resulting in a blindingly fast system for generating 3D structures of crystalline materials.

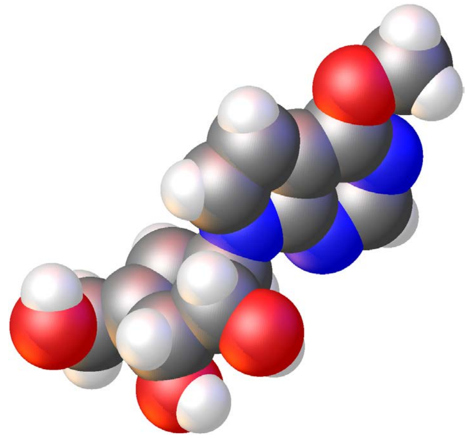

Fig. 3. The structure of the light organic sample shown in space-filling mode.

Table 2. Comparison of the Nova source and the XtaLAB Synergy microfocus Cu source.

Experiment Parameters	SuperNova	XtaLAB Synergy
Crystal to detector distance (mm)	50	52
Exposure time (sec/deg)	1	1
Completeness	97.3	98.6
Redundancy	2.4	2.1
I/sigma to 0.84 Å	25	**39**
Dose time	7 min 5 sec	6 min 29 sec
Rint	0.026	**0.018**
R1 (%)	4.14	**2.74**

3. Applications

If you consider the XtaLAB Synergy not just as made up of these improved individual components; sources, detectors, goniometers, but instead look at the total combined effect, it offers a truly powerful instrument. As a comparison, we can show how the performance is improved against the highly regarded SuperNova in the following applications.

3.1. Comparing the XtaLAB Synergy using similar detector distance

In this example a light, organic compound with orthorhombic symmetry $P2_12_12_1$ (Fig. 3) was compared on both the XtaLAB Synergy and the SuperNova. Similar crystal-to-detector distances were chosen and the same data collection speed was used. With the fixed variables, this example is a good test of the power of the Cu PhotonJet source.

As shown in Table 2, the XtaLAB Synergy PhotonJets provide more than a 50% increase in I/σ compared to the SuperNova. The improvement in I/σ subsequently means that the Rint and R1 of the final structure are considerably lower.

Table 3. Results of three comparative experiments on the XtaLAB Synergy vs the SuperNova.

Experiment parameters	SuperNova	XtaLAB Synergy Very fast	XtaLAB Synergy using extra data
Crystal to detector distance (mm)	50	35.5	35.5
Completeness to 0.84 Å	99.2	98.6	99.8
Redundancy	2.7	2.1	2.7
Relative goniometer speed	×1	×2	×2
I/sigma to 0.84 Å	26	39	59
Experiment time	12 min 48 sec	7 min 38 sec	11 min 17 sec
Rint	0.036	0.018	0.016
R1 (%)	3.97	2.74	2.54

3.2. The overall improvements of the XtaLAB Synergy

In the second example, data was collected on the same sample as above, but this time to compare the combined speed of the XtaLAB Synergy versus the SuperNova. Three data sets were collected with the first two designed to go as fast as possible on each of the aforementioned system. The biggest differences in the experiments were the minimum crystal to detector distance and the speed of the goniometer as shown in Table 3. In the third experiment, the extra time saved by the efficient XtaLAB Synergy was used to collect better quality data.

These results highlight the benefits of the new, faster goniometer, the closer detector distance and increase in source flux of the microfocus source.