

Chemical Crystallography

Single crystal X-ray diffraction

Systems designed for small molecule crystallography



Rigaku
oxford diffraction

Rigaku Oxford Diffraction

THE POWER OF SYNERGY

Combining the best cutting-edge hardware components with highly parallelized software creates a synergistic effect that results in fast, powerful diffractometers for tackling the hardest of problems in chemical crystallography.



XtaLAB mini II



XtaLAB Synergy-S



XtaLAB Synergy-R



XtaLAB Synergy-DW

CrysAlis^{Pro}

At the nerve center of every Rigaku Oxford Diffraction chemical crystallography diffractometer lies CrysAlis^{Pro}, one of the world's most popular data collection and processing packages. CrysAlis^{Pro} is often referred to as "user-inspired software," in that Rigaku Oxford Diffraction's software team makes a concerted effort to incorporate features and functionality based on our customers' ideas and feedback.

CrysAlis^{Pro} runs all hardware and software modules in parallel to achieve the highest efficiency and speed. This design maximizes instrument use by automating mundane tasks, allowing more time to address the difficult problems that today's crystallographers face.

CrysAlis^{Pro} combines automated crystal screening, the fastest and most accurate strategy software available, concurrent data reduction and automatic structure solution with refinement by AutoChem, giving visual feedback in the shortest time possible. CrysAlis^{Pro} can be run in an automated mode but experts can just as easily run in a manual mode with access to a rich collection of software tools.

Routine crystal samples can, of course, be handled quite easily, but a wide range of more challenging problems can be tackled using the tools included as part of CrysAlis^{Pro}, including

- Twinned crystals, incommensurate structures, and quasi-crystals.
- High-pressure data collection with strategy and data reduction optimized for diamond anvil cells.
- Multi-temperature and multi-wavelength experiments.
- Powder diffraction experiments.



XtaLAB mini™ II

THE PERFECT TEACHING AND RESEARCH TOOL

The XtaLAB mini II benchtop X-ray crystallography system is designed to produce publication-quality crystal structures. The simple design makes it the perfect system for teaching single crystal analysis in an academic setting, as well as for use directly in a synthetic chemistry lab as a tool for quick structure determination.

Equipped with a Mo sealed tube source running at 600 W, focusing optics, and an extremely low noise HPC (Hybrid Photon Counting) detector, the XtaLAB mini II is a minimal maintenance system capable of collecting research level data.

Unique benefits of the XtaLAB mini II

- Benchtop diffractometer providing publishable quality results.
- User-friendly and semi-automated.
- Robust enough for students to operate in a teaching environment.
- Latest low noise HPC detector technology.
- Researcher and student friendly, comprehensive CrysAlis^{Pro} software.



The XtaLAB mini II diffractometer.

FEATURES

- Essentially noise-free HPC detector with 100 μm pixels.
- Robust, simple design with a small footprint.
- Sealed tube molybdenum X-ray source with focusing optics.
- Compatible with a Cryostream 800 low temperature attachment.
- Research quality data, exceeding IUCr standards.
- Compact, fail-safe radiation enclosure.

The XtaLAB mini II has just three moving parts: the shutter and the phi and omega axes of the goniometer. The latter of these were designed specifically for ease of mounting – useful when training new users. The simple design also means minimal maintenance and no special infrastructure requirements, important for universities or service laboratories with limited budgets.

XtaLAB Synergy S – A Crystallographer’s Dream Co

DESIGNED FOR DATA QUALITY AND SPEED

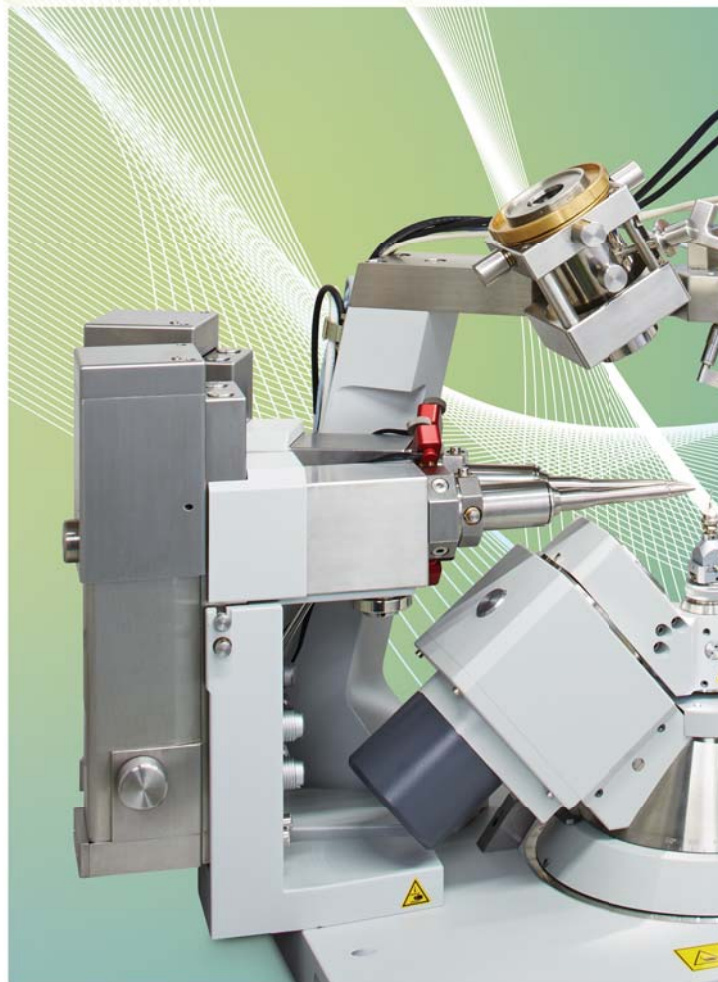
The common goal of any single crystal experiment is to efficiently and accurately measure reciprocal space data. This is true whether you are determining the structure of a novel chemical compound, screening a crystal before a synchrotron trip or measuring highly redundant, high-resolution data for a charge density study. In all cases, the quality of the data generated by your diffractometer, as well as the speed and ease by which you can measure the data, is paramount to the productivity of your research. With your success utmost in our mind, we have produced the XtaLAB Synergy-S diffractometer, a combination of leading edge components and user-inspired software tied together through a highly parallelized architecture to produce fast, precise data in an intelligent fashion.

The XtaLAB Synergy-S is comprised of one or two PhotonJet-S X-ray sources (Mo, Cu, or Ag), a high-speed kappa goniometer, an HPC detector, and an ergonomically designed radiation enclosure.

In addition to Rigaku’s HyPix-6000HE detector, selected Dectris PILATUS HPC detectors are supported by the XtaLAB Synergy-S, such as the PILATUS3 R 300K, and PILATUS3 R CdTe models.

Unique benefits of the XtaLAB Synergy-S

- Extremely powerful and tightly stabilized X-ray source for best, consistent performance.
- Highest throughput sealed tube diffractometer available.
- Class leading results in all applications.
- Extremely low noise photon counting detector.
- Researcher and student friendly, comprehensive CrysAlis^{Pro} software licenses.



FEATURES

- PhotonJet-S X-ray sources utilize the latest in microfocus X-ray sources, newly designed multilayer optics as well as improved alignment.
- The speed of the goniometer has been improved and now reaches 10°/sec.
- The default detector for the XtaLAB Synergy-S is the HyPix-6000HE, featuring near zero dead-time, extremely low noise and 100 Hz frame rate.
- AutoChem 3.0 is included with every XtaLAB Synergy-S. One of the features of AutoChem 3.0 is the “What is this?” tool – a feature that allows you to determine your structure in advance of the complete data collection.
- Electronically controlled brightness of cabinet and crystal for all types of crystal samples.
- No need for an external water chiller, which reduces maintenance.
- Online diagnostics and troubleshooting enhances the ability of service engineers.

ome True



us sealed X-ray tube technology and incorporate alignment mechanisms.

ow allows data collection scan speeds of up to

HyPix-6000HE, an HPC detector with 100 μm pixels, frame rate.

S diffractometer. One of the most powerful features that allows you to rapidly collect enough data to data collection.

al lighting results in optimal video images

maintenance.

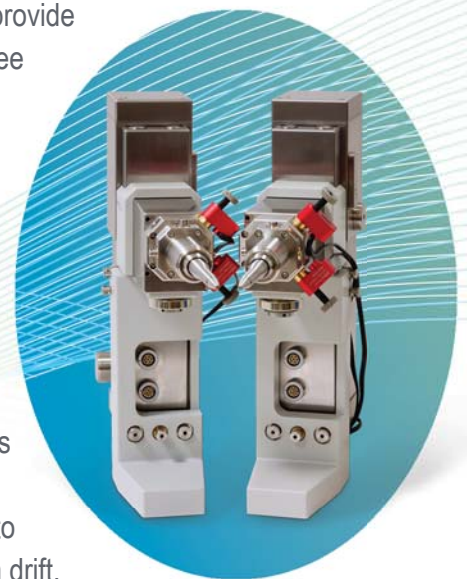
bility to diagnose and fix problems by remote

PhotonJet-S

At the heart of every XtaLAB Synergy-S is the new PhotonJet-S X-ray source. Based on a new microfocus sealed tube design, engineered specifically for single crystal research, the PhotonJet-S incorporates a new mirror design and new alignment hardware.

The new PhotonJet-S sources provide almost double the flux for all three target types compared to the previous model.

A key feature of the PhotonJet-S source is a special internal cooling circuit that maintains the anode temperature within a strict tolerance. With microfocus tubes it is important that the anode be kept at a constant temperature to eliminate the possibility of beam drift.



HyPix-6000HE[†]

The features of the new HyPix-6000HE detector provide many benefits for measuring single crystal data. This is a direct detection detector that requires no phosphor. The point spread function of a reflection is determined by the pixel size rather than from phosphor blooming. A 100 μm pixel thus reduces the size of reflections and minimizes reflection overlap, and also minimizes the area in which background will be accumulated.

The 100 Hz frame rate, near zero dead time and extremely low detector noise lead to true shutterless data collection. Another powerful feature is the ability to reduce fluorescence background by setting the appropriate energy threshold.



[†] This product was jointly developed by Department of Measurement and Electronics, AGH University of Science and Technology (Poland) and Rigaku Corporation.

Extremely small samples or high-throughput needs?

HIGH-FLUX ROTATING ANODE MODELS

Increasing the X-ray flux on your sample has two benefits. For extremely small samples, additional flux will extend the minimum size limits for crystals that you can study. For labs with high-throughput requirements, increasing the flux will reduce data collection time and thus increase the number of samples that can be studied in your laboratory. Rigaku Oxford Diffraction produces two XtaLAB models that are based on the highly reliable MicroMax-007 HF rotating anode generator. These systems provide up to a 10-fold improvement in flux at the sample compared to microfocus sealed tube sources.

XtaLAB Synergy-R

The new XtaLAB Synergy-R is similar to the XtaLAB Synergy-S except that the PhotonJet-S X-ray source has been replaced by a PhotonJet-R X-ray source. The foundation of the PhotonJet-R X-ray source is the MicroMax-007 HF microfocus rotating anode generator with a newly designed optic to complement the geometry of the Synergy. The PhotonJet-R is coupled directly to the kappa goniometer and the alignment mechanism has been designed for easy maintenance. Available with a Cu, Mo or Ag anode.

Unique benefits of the XtaLAB Synergy-R

- Extremely powerful small molecule diffractometer.
- Provides unparalleled throughput.
- Excels at the most challenging applications (MOFs, charge density...).
- Extremely low noise photon counting detector.
- Researcher and student friendly, comprehensive CrysAlis^{Pro} software licenses.



The XtaLAB Synergy-R.

XtaLAB Synergy-DW

The flexibility of having multiple wavelengths to choose from when designing an experiment can also be achieved with a high-flux diffractometer. Instead of incorporating two X-ray sources with different targets, the XtaLAB Synergy-DW diffractometer utilizes a double banded anode, a dual multilayer optic assembly, and an easy mechanism for switching between two wavelengths.

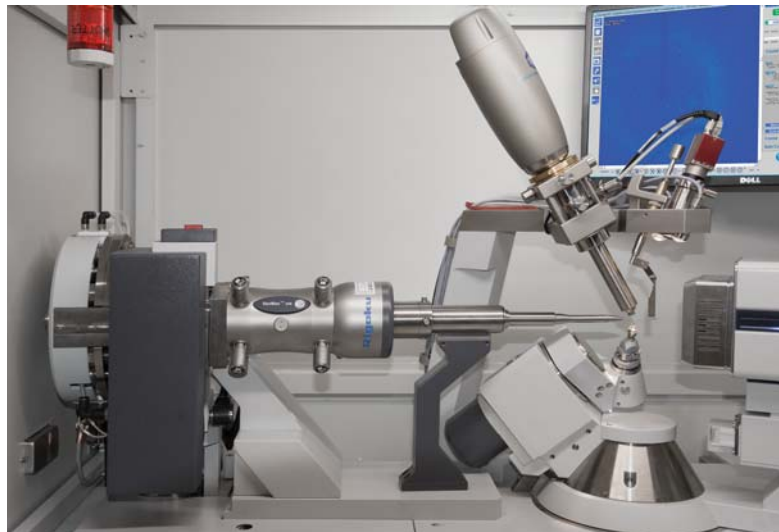
- Available with a variety of anode material combinations, such as Cu/Mo, Cu/Cr, etc.
- Switching between anode types is easily accomplished in five minutes.

XTALAB SYNERGY CUSTOM

The Synergy goniometer can be configured in numerous ways with Rigaku's rotating anode sources to fit the needs of any lab.

- The second port of the X-ray source can easily be utilized to mount an additional goniometer with a custom enclosure.
- A larger rotating anode source, the FR-X, provides more than double the flux of the MicroMax-007 HF and can be configured with a number of goniometer and detector combinations.
- For the ultimate in charge density applications, a Ag version of the MicroMax-007 HF is available to be coupled with a PILATUS3 R CdTe detector.

Dual Wavelength Rotating Anode



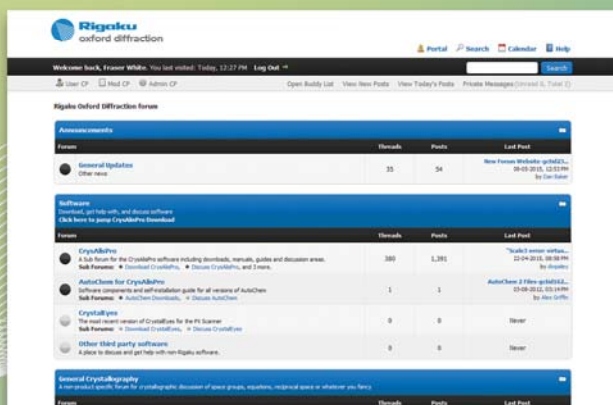
Close up view of the DW anode shifting mechanism and dual wavelength optics assembly.

Unique benefits of the XtaLAB Synergy-DW

- Combines the increased flux that can be obtained from a rotating anode X-ray source with the flexibility of being able to switch between two different wavelengths.
- The switch between wavelengths is accomplished in only five minutes.
- It is not necessary to perform any realignment after switching from one wavelength to the next.
- Overall maintenance is reduced since only one generator is required for two wavelengths.
- The perfect system for laboratories that work with extremely difficult samples that need the enhanced flux of rotating anode sources, as well as those that have a large array of samples that can benefit from having Mo and Cu available for structure analysis.

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Chemical Crystallography

Single crystal X-ray diffraction

www.Rigaku.com
www.Rigaku-OD.com

**Your Success
is Our FOCUS**

The employees of Rigaku Oxford Diffraction are dedicated to providing the best solutions for single crystal analysis, whether it be small molecule or macromolecule related research. Our inspiration comes from helping you solve your difficult experimental problems and our personal satisfaction derives from helping you achieve your research goals.

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