Agilent Xcalibur and Gemini X-ray Diffractometers

ENHANCED CHEMICAL CRYSTALLOGRAPHY SOLUTIONS

The Measure of Confidence

Agilent Technologies

ENHANCED CHEMICAL CRYSTALLOGRAPHY SOLUTIONS

Agilent's Xcalibur and Gemini single-crystal X-ray diffractometers have a proven track record earned over many years. From the first Xcalibur—installed in 1999—to the world's first co-mounted dual-source diffractometer, the Gemini (2005), both instruments have well-deserved reputations for providing great data quality, with outstanding system reliability.

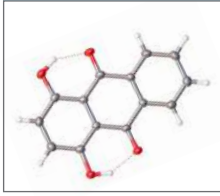
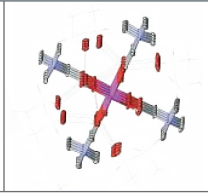
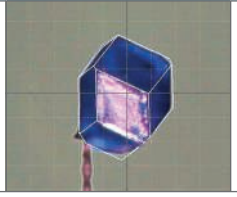
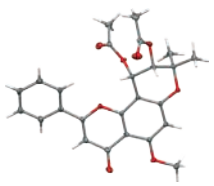
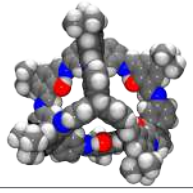
Our new Xcalibur and Gemini systems incorporate the best features from their predecessors, whilst now benefitting from the very latest, state-of-the-art electronics, as well as an enhanced protection cabinet with our innovative *motion enable* system. With these improvements, you can be confident that your system is able to handle the ever-increasing demands of the modern day laboratory environment.

Dual source Gemini X-ray diffractometer with Eos S2 CCD detector.

New Xcalibur and Gemini System Features

- Enhance fine-focus X-ray sources with monocapillary optics – Single or dual-wavelength
- Easy dual-source Gemini upgrade
- 4-circle kappa goniometer
- Accepts full range of S2 CCD detectors and cryo-devices
- New protection cabinet with *motion enable* system – Fully compliant with EU safety directives
- Compact – Ideal for space-limited laboratories
- Single, high voltage generator
- Enhanced diagnostic firmware for improved service and support
- Powerful external PC for instrument and experiment control
- CrysAlis^{Pro} – Powerful, user-friendly software, with optional AutoChem$^{2.0}$ for fully-automated structure solution and refinement

Applications

Service	Extended inorganics	Strongly absorbing materials	Absolute structure	Macro-molecules	Small/weakly diffracting crystals
					

CUSTOMIZABLE SINGLE AND DUAL SOURCE SYSTEMS

Configure your system for specialist applications as well as for multi-disciplinary laboratories.

Fine-focus X-ray Sources

Up to 3kW Mo and 2.2kW Cu Enhance X-ray sources: Your choice of single or dual wavelength system, or upgrade later.

Optional Cryo-devices

Accepts all major open-flow cryogenic devices including Agilent's Helijet liquid helium device; the Cryostream, Cobra and Desktop Cooler from Oxford Cryosystems; and Oxford Instruments' Cryojets.

CrysAlis^{Pro} Software

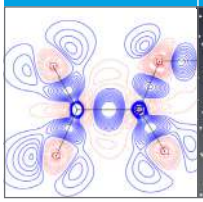
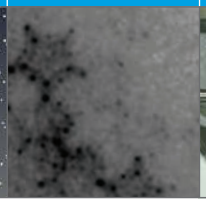
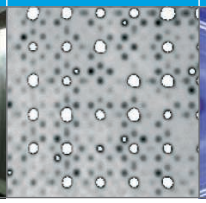
Powerful, user-friendly data collection and data reduction software. Offered under a multi-site, multi-user licence, with **free regular updates** from our dedicated single-crystal programming team.

4-Circle Kappa Goniometer

Precise movement with accurate sample and detector positioning using stepper motors and optical encoder sensors. Theta range significantly higher than IUCr data resolution requirements in all configurations.

S2 CCD Detectors

Unique, self-optimizing CCD detectors. Three options to choose from for size and sensitivity, with an Intelligent Measurement System including Smart Sensitivity Control (SSC) and flexible pixel binning.

Charge/ electron density	Twinning	Quasi-crystals	High pressure	Incom-mensurates	Powder diffraction	Fiber diffraction
						

SINGLE SOURCE XCALIBUR OR DUAL SOURCE GEMINI

Agilent designs systems as complete units and manufactures all main components. With Enhance X-ray sources in production since 2001 and CCD detectors since 1992, Agilent's expertise offers proven performance and reliability.

Enhance X-ray Sources

Xcalibur and Gemini systems employ Enhance fine-focus X-ray sources, which can be either molybdenum or copper radiation and are factory pre-aligned to give maximum intensity. Easy to use, the patented Enhance design comprises:

- A long fine focus ceramic X-ray tube (2.2 – 3 kW)
- Integrated fast X-ray shutter and secondary safety shutter
- Pre-aligned monochromator
- Mono-capillary collimators (0.3 – 1.0 mm available), changeable by hand in only a few seconds

Enhance X-ray sources are cooled by an external water chiller, which can be linked to a dedicated laboratory cooling circuit or standalone water-to-air chiller.

Single source Xcalibur configuration, with Eos S2 CCD detector.

Dual source Gemini configuration (Cu at the front and Mo at the back), with Eos S2 CCD detector.

At the Sample Position

- 4-circle kappa geometry offers greater flexibility, more efficient data collection strategies and higher overall completeness.
- The single or dual beamstop can be moved away from the sample position, for better use of cryo-tools.
- A video microscope providing 120x total on-screen magnification is used for accurate sample centring. A movie of every sample measured is collected as part of every dataset.
- Cool, focusing LEDs light the sample position, enabling high-clarity sample visualisation without any effect on fine sample temperature control.

Dual Source Upgrades

- Single source Xcalibur systems can benefit from an on-site upgrade to a dual-source Gemini configuration at any later date

UNIQUE, SELF-OPTIMIZING S2 CCD DETECTORS

Eos S2

- Agilent's most sensitive detector – Ideal for all service applications, as well as weak data, charge density, high pressure and incommensurate studies
- Active area Ø 92 mm
- Gain: Up to 400:200 e^-/X-ray (Mo:Cu)
- Truesense Imaging KAF-4320E 2,048 x 2,048 CCD chip
- 0.22 s readout time (4x4 binning)
- Low noise (<12 e^- RMS full frame)
- 18 bit precision (hard wired)
- S2 Intelligent Measurement System, with Smart Sensitivity Control (SSC) and automated, flexible pixel binning

Or Upgrade...

Atlas S2

- Optimum combination of large active area and detector sensitivity for the most efficient datasets
- Active area Ø 135 mm
- Gain: Up to 180:90 e^-/X-ray (Mo:Cu)

Titan S2

- Largest active area means more data per image – Ideal for Cu datasets and larger unit cells
- Active area Ø 165 mm
- Gain: Up to 100:50 e^-/X-ray (Mo:Cu)

S2 Intelligent Measurement System

S2 CCD detectors offer a unique, self-optimizing Intelligent Measurement System, with settings automatically adjusted based on the characteristics of observed data:

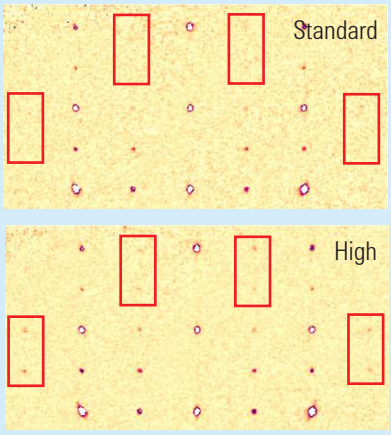
- **Smart Sensitivity Control (SSC)** – State-of-the-art on-board electronics tune detector sensitivity to match the sample being studied. Similar to the ISO setting in digital photography, three SSC settings help to boost weaker data over the background (see right), or offer a wider dynamic range for successful measurement of the strongest data.
- **Flexible Pixel Binning** – S2 detectors are operated in 1x1, 2x2 and 4x4 binning modes. This offers a range of pixel sizes for variable spatial resolution, sensitivity and dynamic range. Switching between modes is instant and automatic in CrysAlis^{Pro}.

Combining SSC with flexible binning offers great flexibility, with settings tuned for weak data, for strong data and for remeasured data, often all in the same dataset.

High Signal-to-Noise and High Speed, without Compromise

High gain and low read noise together mean that S2 CCDs provide optimal signal-to-noise ratios for single crystal data. Plus, 4-port chip technology enables rapid readout times for all S2 detectors – approaching continuous readout – but without negative consequences such as shutter skew, which is a feature of some alternative technologies (e.g. APS CMOS).

Smart Sensitivity Control



High SSC mode can make the difference when observing very weak reflections in like-for-like experiments.

USER-INSPIRED CRYSTALLOGRAPHY SOFTWARE

CrysAlis[Pro] is Agilent's comprehensive data collection and data processing software for small molecule experiments. Designed around an easy-to-use graphical user interface, CrysAlis[Pro] can be operated under fully automatic, semi-automatic or manual control, and incorporates a wide range of sophisticated, intelligent tools for all requirements in chemical crystallography.

Automatic Crystal Screening

At the heart of CrysAlis[Pro] are automatic crystal screening and data collection strategy modules. For a typical crystal, a very short pre-experiment is recorded to evaluate crystal quality. From the first image, CrysAlis[Pro] automatically determines diffraction quality and provides the user with the unit cell, intensity estimation by resolution range and suggested exposure times for a full data collection. CellCheckCSD (developed with the CCDC) automatically screens the Cambridge Structural Database for unit cell matches to prevent the collection of known structures.

Fast, Efficient Data Collection Strategies

CrysAlis[Pro]'s sophisticated strategy software automatically calculates the optimal conditions for fast, high quality, complete data collection regardless of wavelength. Strategies take seconds to compute and can be optimized for multiplicity, coverage, time, resolution and many other criteria, including working with high pressure diamond anvil cells (DACs).

Automatic and Concurrent Data Reduction

Data reduction begins at the start of data collection and employs intelligent routines which tune the parameters for optimum data quality. Principle corrections (incl. absorption, frame scaling) are always applied automatically, and processed data are accompanied by real time on-screen feedback. CrysAlis[Pro] is programmed for multi-core data processing, meaning rapid results even from the largest data sets.

Compatibility, Updates and Licensing

CrysAlis[Pro] imports and processes images from other detector formats, with data easily exported for use in third-party data reduction packages. The software interfaces directly to Olex2, SHELX, CRYSTALS, WinGX, Jana and CCP4.

CrysAlis[Pro] updates offer every user access to the very latest developments. The software and all future updates are provided **free of charge** to all Agilent system users under a multi-user, multi-site license.

Comprehensive Tools

- Advanced peak hunting & unit cell finding
- Ewald[Pro] reciprocal lattice viewer
- Flexible data processing and data optimization tools
- Interactive space group determination
- Automated face-indexing
- Absorption correction utility
- Twin/Incommensurate/Quasi-crystal data processing
- High pressure data collection/ processing
- Multi-temperature/wavelength setup
- Powder diffraction experiments
- Precession images and axial photos

AUTOMATED STRUCTURE DETERMINATION

The ultimate productivity tool for chemical crystallography, AutoChem2.0 works seamlessly with CrysAlisPro offering fast, fully automatic structure solution and refinement during data collection. See your structure long before the experiment is complete, without any manual intervention.

Seamlessly Integrated with CrysAlisPro

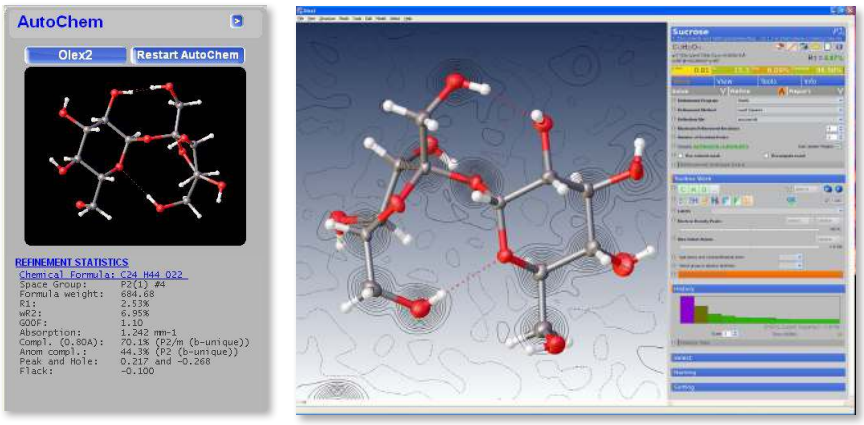
Developed exclusively for Agilent by the authors of Olex2 (Durham University and OlexSys Ltd.), AutoChem2.0 builds upon the strength of Agilent's original AutoChem software. Seamlessly integrated as an optional plug-in for CrysAlisPro, AutoChem2.0 offers an advanced approach for automatic structure determination, with an even higher rate of success.

User Input, Structure Solution and Refinement

AutoChem2.0 can work with or without a chemical formula, intelligently using multiple solution programs and typically requiring only partial completeness to solve routine structures. In more difficult cases, AutoChem2.0 will make attempts in multiple space groups. A number of refinement options are available; atoms are modelled anisotropically where the data supports this approach and hydrogen atoms are included in calculated geometric positions. The structure is then re-labelled and refined to completion before a final structure report is generated.

Manual Control

CrysAlisPro displays the structure and key refinement parameters, and provides a link to a full Agilent edition of Olex2 — complete with AutoChem2.0 plug-in — which can be launched at any time. Here the user can review all aspects of the refinement, step back to any stage of the process and apply changes as necessary.



AutoChem2.0 shown during data collection in CrysAlisPro (left), with a seamless link to Olex2 (right).

AutoChem2.0 Features

- Fully automated structure solution, refinement and report generation in real time
- Intelligent structure solution using SMTBX (olex-solve), SHELX, SIR or Superflip (local licenses permitting)
- Can work with or without providing a chemical formula
- Generates solutions in multiple space groups in difficult cases
- Fourier-type atom assignment
- Developed using >2500 structures
- Full user interaction and intervention possible at anytime in Olex2
- AutoChem2.0 is exclusive to Agilent

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