Gemini A
Dual Wavelength Diffractometer for Small Molecule Crystallography

Application Note

X-ray Crystallography

Introduction

The Gemini A is the ideal X-ray system for today's modern small molecule crystallography laboratory.

Designed and brought to you by the world's leading manufacturers of dual wavelength systems, the Gemini A has been designed as a compact and easy-to-use instrument combining the versatility and benefits of co-mounted both molybdenum and copper Enhance X-ray sources on a single 4-circle kappa goniometer.

Agilent Technologies

Co-Mounted Mo and Cu X-Ray Sources

At the heart of the Gemini A is the Agilent original dual wavelength design. The Gemini A combines the patented copper and molybdenum wavelength Enhance X-ray sources which are co-mounted on a single kappa goniometer. Both X-ray sources incorporate mono-capillary optic collimators, graphite monochromators and easy change high precision fast X-ray shutters. The Agilent patented design of Enhance X-ray source gives up to 2.5× more flux than a traditional small molecule sealed tube and are extremely easy to maintain. Pre-aligned in the factory, the X-ray tube exchange takes only a few minutes and requires minimal or no re-alignment.

CCD Detector

The Gemini A incorporates the 135 mm Atlas CCD detector which uses the highest quality 2K × 2K Kodak CCD providing an extremely high detective quantum efficiency. The true 18-bit dynamic range of the hardware, coupled with the high sensitivity of the Atlas CCD, means that the Gemini A is optimised for measurement of weak and strong peaks in the same image and is ideal for small molecule crystallographic studies with both Mo and Cu wavelength radiation.

Figure 1. 4-circle kappa Gemini platform fitted with an Atlas CCD detector and co-mounted molybdenum Enhance and copper Enhance X-ray sources.

Platform

The Gemini A is built around the Agilent high precision 4-circle kappa goniometer which allows the collection of high quality, high resolution data with both molybdenum and copper radiation. The sample to detector distance is software controlled and motorised over the range 40–150 mm enabling the resolution of unit cells of up to 500 Å. For cryogenic cooling of the crystal sample the platform is compatible with a range of devices including the Cryojet open flow nitrogen cooler (490K–90K) and the patented Helijet open flow helium cooler (90K–10K).

Figure 2. The co-mounted Enhance (Mo) and Enhance (Cu) X-ray sources.

Software

The Gemini A is supplied with the Agilent comprehensive software called CrysAlis^{Pro} which is a fully automated package for trouble free small molecule data collection and reduction.

Automatic Screening, Data Collection and Data Reduction

CrysAlis^{Pro} features automatic data collection, screening and sophisticated strategy software. A typical experiment involves the collection of 15 data frames. From the first frame auto-evaluation of the crystal quality begins. This includes unit cell determination, I/sigma estimation by resolution range and the determination of the crystal Laue class. Following the auto-screening CrysAlis^{Pro}'s strategy module calculates the optimal data collection experiment and frame exposure time for the crystal.

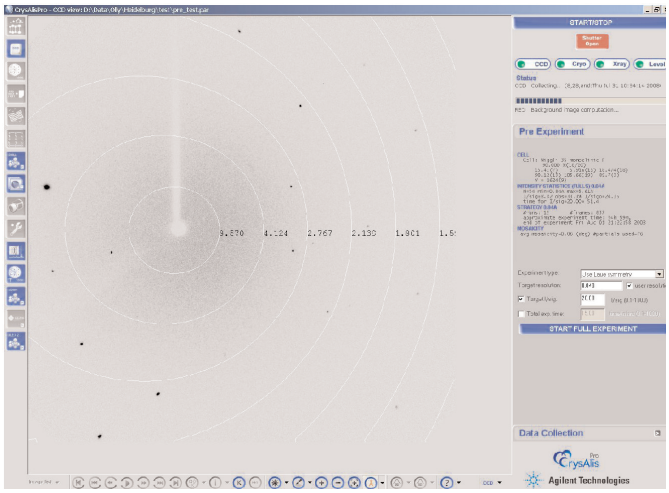

Figure 3. Screenshot of CrysAlis^{Pro}.

Data Collection Strategy

CrysAlis^{Pro}'s automatic strategy module allows the user to optimise the data collection for completeness, multiplicity, time, resolution, detector distance and crystal Laue class. The combination of the strategy software and the 4-circle kappa geometry makes for faster, more complete data collection and uniquely allows data collection to be optimised for the measurement of anomalous pairs on the same image.

Concurrent Data Collection and Reduction

Data reduction is concurrent with data collection and is intelligent, auto-tuning parameters for the best data quality and making it the easiest to use software for both small molecule and protein crystallography. The concurrent data reduction means that processed data is always available, accompanied by up to the minute on-screen feedback of the data quality and completeness statistics.

Specialist Crystallographic Tool

CrysAlis^{Pro} also provides a wide range of specialist crystallographic tools. These include tools for visualisation of reciprocal space, twinning, space group determination and remote control of the X-ray generator, Cryojet and liquid nitrogen auto-fill, all of which are automatically logged for the duration of the data collection.

Third Party Compatibility and Software Licences

CrysAlis^{Pro} provides data in HKL and MTZ format and interfaces easily to SHELX, CCP4 suite and third-party data reduction packages including MOSFLM, XDS and HKL2000. It is provided under a multi-site, multi-user licence with free upgrades.

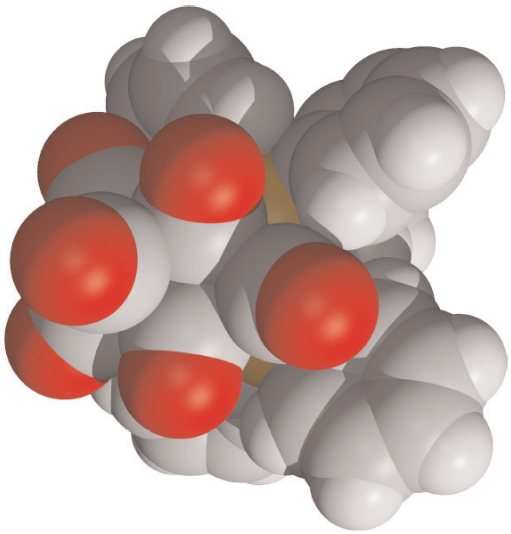

Figure 4. An example small molecule crystal structure.

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