CHEMICAL CRYSTALLOGRAPHY

D8 QUEST
D8 VENTURE

High-End Solutions for X-ray Crystallography

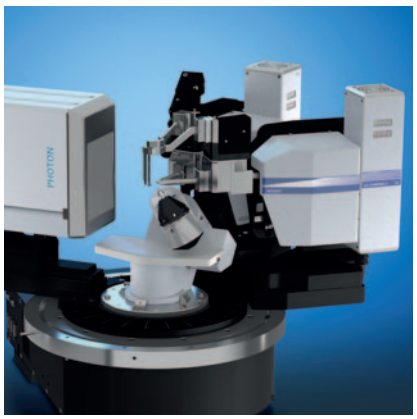
Innovation with Integrity

IμS DIAMOND II: Rotating anode performance

LED enclosure illumination

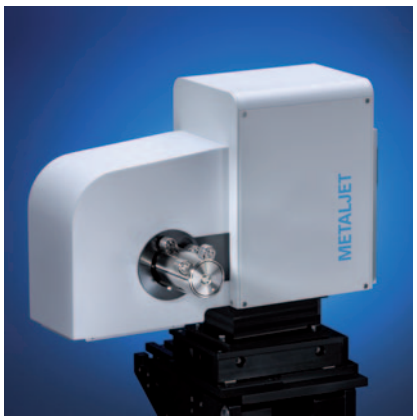
Low temperature attachment

Compact IμS 3.0 microfocus source



Stable and easy-to-align beam path

Wide doors for easy access



METALJET D2 PLUS:
the most intense home source

Large area PHOTON III charge-integrating pixel array detector


BRUKER
D8 QUEST
BRUKER
D8 VENTURE
METALJET

Crystallography: Driving modern science

Detailed insight into the relationship between molecular structure, function, and reactivity is crucial for the success of modern chemical science. Crystallography is one of the most powerful methods for generating this vital information and has thus become an essential tool for new discovery.

The great importance of crystallography – in chemistry, biology, pharmacology, mineralogy, physics and other areas of research – is illustrated by the fact that 29 Nobel prizes have been awarded within this field.

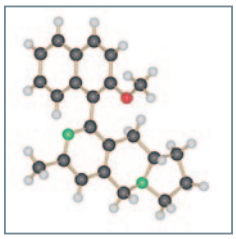
Great Science Deserves Great Tools

As the frontiers of science advance, the need for better structural data is growing more acute and therefore modern laboratories need better crystallographic instruments – with more power, more speed and better ease of use.

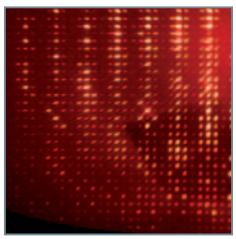
At Bruker, our driving passion is to provide scientists with the best tools for crystallography. In order to achieve this goal, our research and development team has undertaken a broad, six-year development program to push the frontiers of detector and source technology and to expand the possibilities of crystallographic software. Finally, the culmination of this intensive effort is now at hand:

The D8 Crystallography Solutions – D8 QUEST and D8 VENTURE

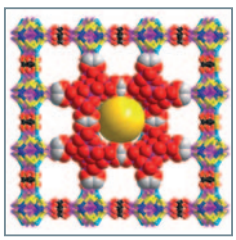
Absolute configuration [1)]



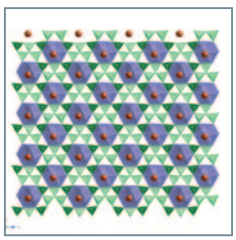
Incommensurate structures [4)]



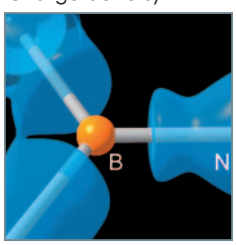
Service crystallography [7)]



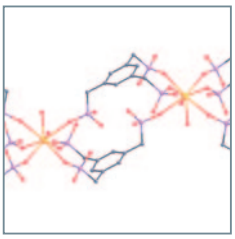
Strong absorbers [10)]



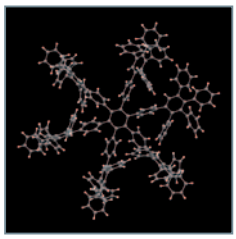
Charge density [13)]



Supramolecular / MOF [2]

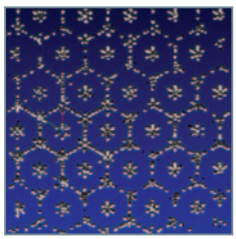


Organic [3]

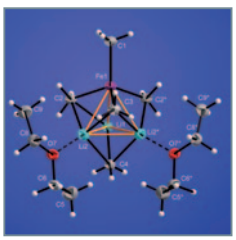


Phase transition [5]

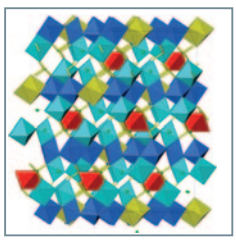
Twinning [6]



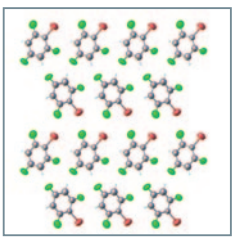
Coordination [8]



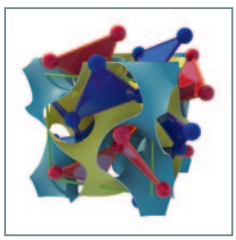
Minerals [9]



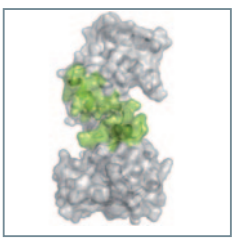
High pressure [11]



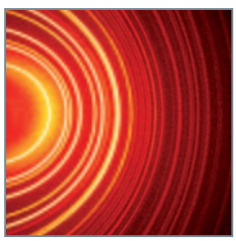
Inorganic [12]



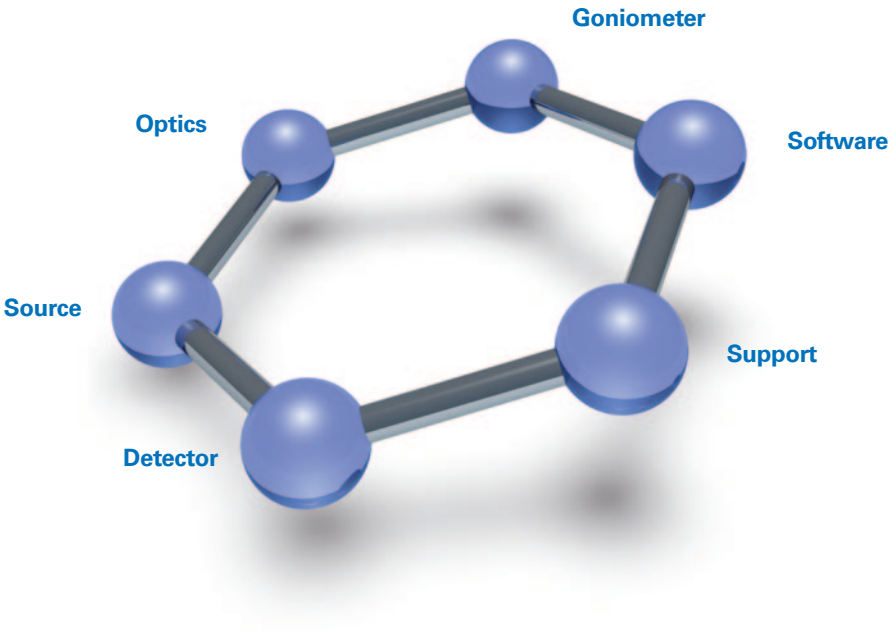
Proteins [14]



Powder [15]



1) Fischer, F; Weding, N; Ott, H; Hapke, M: Publication in preparation
2) Almeida Paz F A , et. al: Chem. Commun., 2013, **49**, 6400
3) Bauer, R E; Enkelmann, V; Wiesler, U M; Berresheim, A J; Müllen, K: Chem - Eur. J., 2002, **8**, 3858
4) Ruf, M; Olmstead, M; Wagner, T; Schönleber, A: New Software Tools for Indexing and Processing of Modulated Structures, 2008 Meeting of the American Crystallographic Association, Knoxville, TN
5) Ali, N Z; Nuss, J; Sheptyakov, D; Jansen, M J: Solid State Chem., 2010, **183**, 752–759
6) Straver, L: Pseudo-merohedral twinning –How to treat a six-fold twin (Bruker Appl. Note, Delft, 2007)
7) Yang, Y C; Wang, S L: J. Am. Chem. Soc. 2008, 130, 1147;Science (Editor's Choice), 2008, **319**, 387–388
8) Furstner, A; Krause, H; Lehmann, C W: Angew. Chem. Int. Ed. 2006, **45**, 440–444
9) Yang, Z; Giester, G; Ding, K; Tillmanns, E: Eur. J. Min. 2011, **23**, 63–71
10) Wang, S; Alekseev, E V; Depmeier, W; Albrecht-Schmitt, T E: Inorg. Chem. 2011, **50**, 2079–2081
11) Probert, M R; Yiu H P; Chung, Y H P; Howard, J A K: Crys. Eng. Comm. 2010, **12**, 2584–2586
12) Nuss, J: MPI for Solid State Research, private communication
13) Flierler, U; Leusser, D; Ott, H; Kehr, G; Erker, G; Grimme, S; Stalke, D: Chem. Eur. J. 2009, **15**, 4595
14) Bolanos-Garcia, V M ; Chirgadze, D Y; Blundell, T L: 2011, BUBR1 kinase, private communication
15) He, B B: Two-Dimensional X-ray Diffraction, Wiley, New Jersey, 2009, **387**



An instrument you can rely on: Today and tomorrow

For many years, the vast majority of published structures have been determined using Bruker equipment. There is a good reason for this: from the X-ray source, through the goniometer and detector, to the analytical software, you always get best-in-class solutions for all of your applications.

X-ray Sources and X-ray Optics

A successful diffraction experiment starts with an excellent X-ray source. Whether you choose an IμS 3.0 microfocus source, the even more powerful IμS DIAMOND II or the ultimate brilliance of our high-end METALJET D2 PLUS source, you always get the best performance.

Goniometer and Sample Stages

Ultimate precision, it's as simple as that: our mechanics are so precise that the sphere of confusion is unsurpassed by any other goniometer, period. Even your tiniest microcrystals stay reliably in the center of the X-ray beam.

Charge-Integrating Pixel Array Detectors

From the company that brought you the first in-house CCD and CMOS detectors, Bruker once again spearheads X-ray detector development with the revolutionary new PHOTON III. The photon-counting PHOTON III detector is available with three different active-area sizes. It employs large monolithic active-area sensors with ultra-low noise, delivering the same cutting-edge technology developed for X-ray Free Electron Laser (XFEL) beamlines. The PHOTON III features an unprecedented combination of large active area, photon-counting sensitivity, and high speed.

Software

Our excellent hardware is complemented by our APEX4 software suite, the world's most advanced software for both instrument operation and data processing. The unique and highly efficient path planning software, based on the latest robotic trajectory algorithms, allows you to make the most of our highly flexible goniometers. It also makes experiment planning easier, faster and more efficient than ever. Data integration, scaling, structure solution, completion and refinement also have powerful software solutions – including the power and convenience of STRUCTURE NOW, our automated data processing software, which will set the standard for the next decade.

Our Best-Structure Guarantee – Only from Bruker!

Good Diffraction Practice: Your safety is our top priority

D8 Crystallography Solutions are designed to the most stringent safety standards.

The typical radiation leakage outside the enclosure is more than an order of magnitude lower than EURATOM regulations!

Two independent fail-safe circuits monitor the safety of the system to prevent any accidental radiation exposure, in compliance with the strictest and most recent radiation and personnel safety regulations.

Furthermore, all warning and operating elements are ergonomically installed, clearly visible, and coordinated with one another in an elegant, state-of-the-art design.

Design, development, manufacturing, and installation of our systems fully comply with ISO 9001:2008. Finally, D8 Crystallography Solutions allow easy sample and beam alignment with the enclosure doors closed, eliminating any potential danger from exposure to scattered X-rays during alignment.

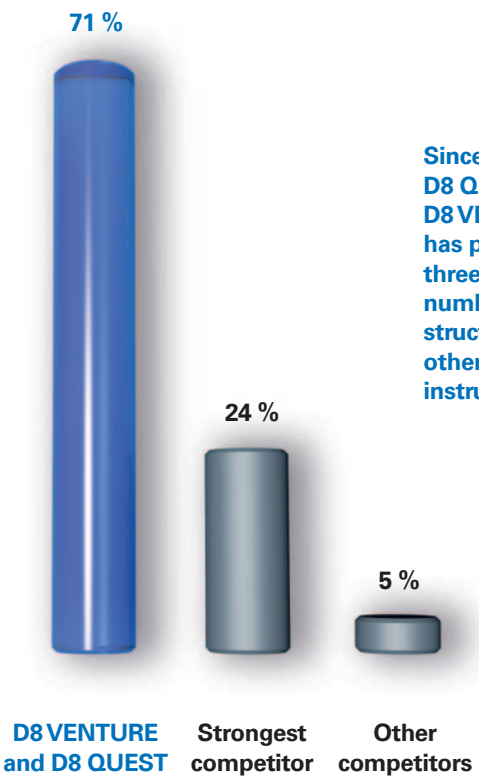
Approved by:

- TÜV
- NEMKO

Conforms to:

- 2006/42/EC
- 2006/95/EC
- 2004/108/EC
- 96/29/EURATOM
- RöV
- DIN EN 954-1 Cat. 3
- DIN EN 61010-1/-2
- CSA C22.2 No. 1010
- EN 61000-6-1/-2/-3/-4

Published Structures in Acta E 2019–2021



Since 2019 the D8 QUEST and D8 VENTURE series has produced nearly three times the number of published structures than other available instrumentation.

The PHOTON III is available in three different sizes, perfectly matching the requirements of your application.

PHOTON III: Charge-integrating, photon-counting detector for superior data

The PHOTON III features the highest Detective Quantum Efficiency (DQE) across the entire energy range typically used in crystallography, up to three times higher efficiency than silicon HPADs.

The best crystal structures for publication require large active-area X-ray detectors with high signal-to-noise ratios for accurate weak- and strong-reflection intensities. Furthermore, high sensitivity for all wavelengths typical for in-house solutions (In, Ag, Mo, Cu, Ga) is essential.

Our PHOTON III detectors match these requirements perfectly:

- The largest active area available in an in-house detector with no gaps or dead areas
- The highest Detective Quantum Efficiency for short wavelength radiation: up to twice the efficiency for Mo radiation and up to three times the efficiency for Ag
- True photon-counting detection for the accurate integration of weak reflections
- Operation in charge-integration mode which eliminates pulse pileup and charge-sharing noise

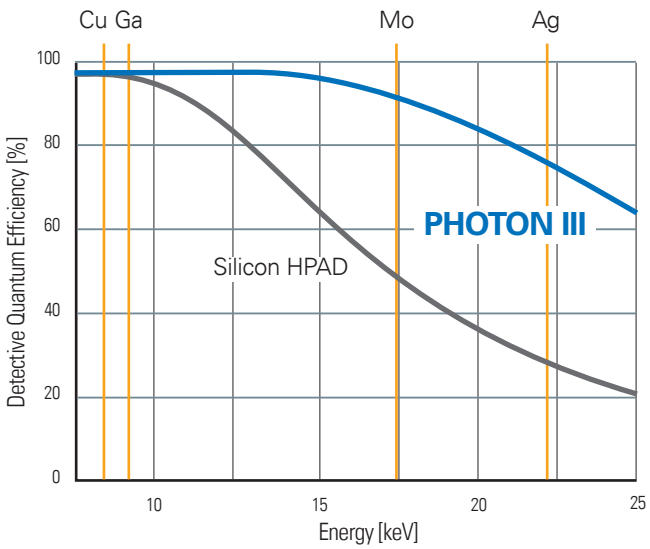
The latest generation of detectors for synchrotrons and XFELs uses a new, improved technique for photon counting based on charge integration. These new charge-integrating detectors, such as the JUNGFRAU (SWISSFEL) and the ePIX (LCLS), do not suffer from pulse pileup or charge-sharing noise and thus have proven to produce markedly superior data compared to conventional Hybrid Photon-Counting (HPC) detectors.

The PHOTON III is the first in-house detector based on this latest charge-integration technology. The PHOTON III features zero detector noise and also eliminates charge-sharing and pulse-pileup noise that plague conventional HPCs.

The PHOTON III also features an advanced rare-earth X-ray convertor that has up to three times the Detective Quantum Efficiency compared to silicon sensors.

The unique combination of features makes the PHOTON III the best in-house detector available.

Absorption efficiency of X-rays



The PHOTON III employs large monolithic sensors and therefore has no dead areas or blind gaps: 100% of the surface is fully sensitive to X-rays.

PHOTON III – Large active-area photon-counting for perfect data

- Largest active area
- Charge integration for best linearity
- Photon-counting for best sensitivity
- High dynamic range
- High Quantum Efficiency over a wide energy range
- Ultra-low parallax
- All air-cooled
- No gaps or dead areas

Best Data

The only laboratory detector with the latest charge-integrating photon-counting technology – excels at both weak and strong reflections, ensuring superior data.

Highest Quality

Three-year warranty, air cooling and no maintenance go hand in hand to deliver a long-lasting, highly reliable detector.

Highest Sensitivity

You can't count what you don't see! Conventional silicon HPC detectors simply miss up to 70 % of the incident X-rays while the PHOTON III sees essentially every photon.

Outstanding linearity

Charge integration means no pulse-pileup noise and thus the best linearity for strong reflections.

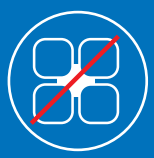
The photon-counting PHOTON III detector delivers outstanding data quality from even the most challenging samples.

Large Active Area

The PHOTON III offers the largest active area for the home laboratory – capture more reflections in just one detector setting and get better separation of closely spaced reflections.

High Speed

With a detector frame rate of 70 Hz, zero readout dead time and shutterless operation, data are acquired quickly and accurately.

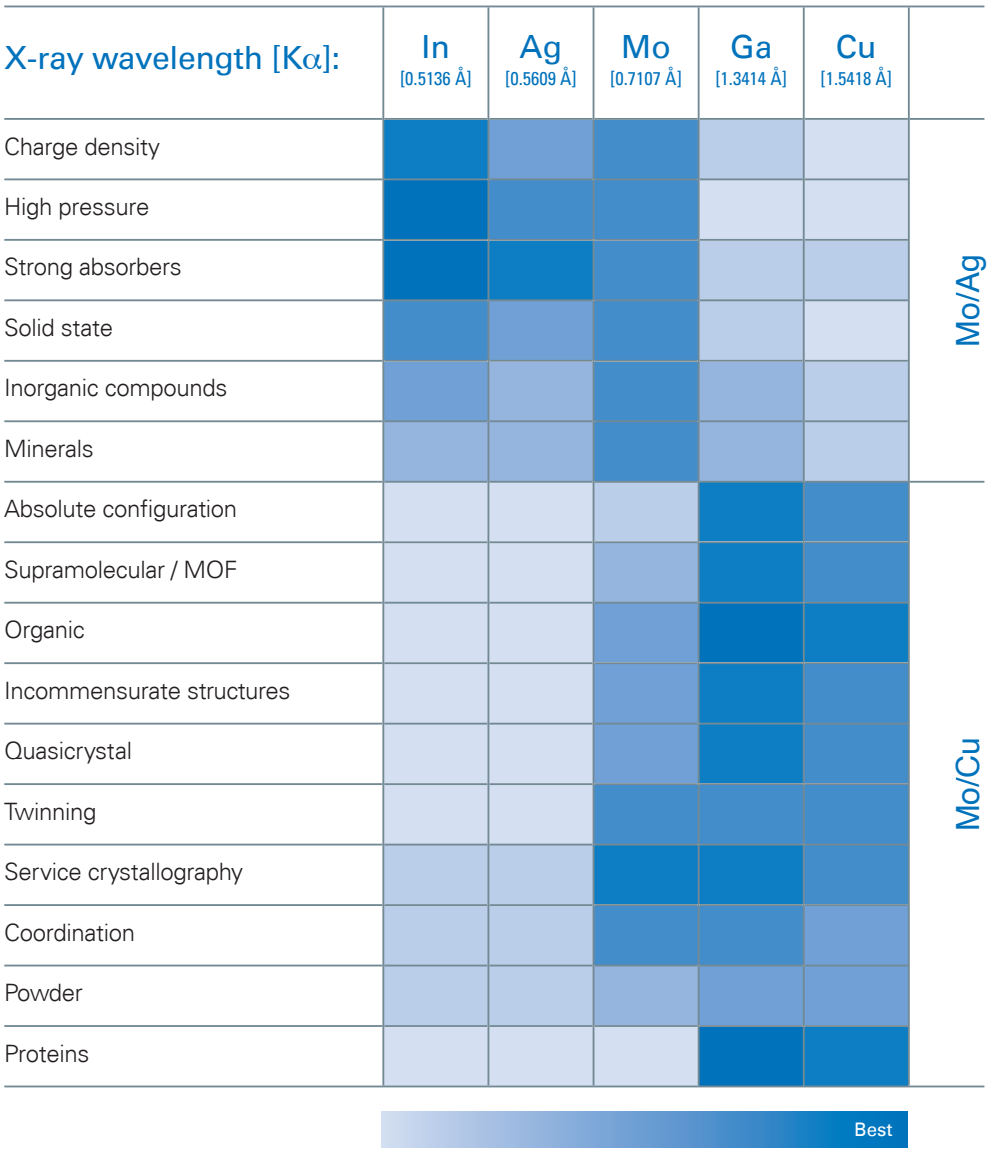


Charge Integration

Charge-integrating detectors record a very high-speed "movie" of the diffraction pattern. A fast processor then looks for X-ray "hits" in each frame of the movie. The result: photon counting with no charge-sharing or pulse-pileup noise for optimal data quality.

Riding the perfect wave

X-ray wavelength suitability



Selecting the right wavelength for your sample can significantly improve the quality of your experiment.

Bruker offers IμS microfocus sources in three standard wavelengths: copper, molybdenum and silver, while the METALJET source is available in gallium and indium wavelengths.

Moly is everybody's darling

With the combination of low absorption, good scattering efficiency and efficient data collection, molybdenum is the traditional favorite of crystallographers and the majority of crystal structures published today use this powerful wavelength. The IμS 3.0 is the most popular source for Mo radiation with more than three times the intensity of competing microfocus sources. The IμS DIAMOND II meanwhile produces the highest intensity Mo beam available in the home laboratory.

Copper: intensity is king

The stronger interaction of copper radiation is ideal for organic samples or smaller crystals. The IμS 3.0 microfocus source with high-performance HELIOS multilayer optics guarantees outstanding intensity that is up to four times higher than competing microfocus sources, while the more powerful IμS DIAMOND II source rivals the intensities of rotating anode sources.

Gallium: "the better copper"

Bruker was the first to integrate the revolutionary METALJET source technology. The METALJET's Ga radiation wavelength is a little shorter than that of Cu. It maintains the proven benefits of Cu radiation and adds several advantages, such reduced X-ray absorption by the sample and reduced scattering by air, thus improving the signal-to-noise ratio. The METALJET delivers all these benefits with an ultra-intense Ga-Kα beam.

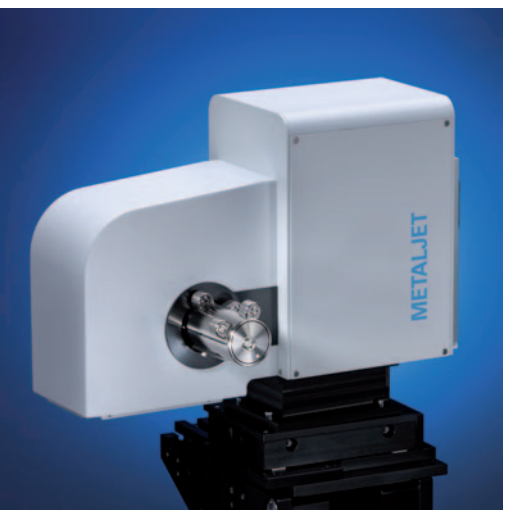
The silver bullet

Silver (Ag) radiation, even shorter in wavelength than Mo radiation, has the benefits of lower absorption and extinction effects, and allows data collection to higher resolution. Diffracted intensities from traditional sealed tubes are very weak, and only with Bruker's introduction of high-intensity Ag microfocus sources has the application of Ag radiation become practical. Advanced deposition techniques have finally perfected high-performance silver (Ag) multilayer optics that are ideally matched to the IμS microfocus source. Ag IμS 3.0 systems produce a small, high-performance beam, which again is topped by the ultra-brilliant IμS DIAMOND II. Both sources provide extensive benefits for solid-state compounds and charge-density experiments.

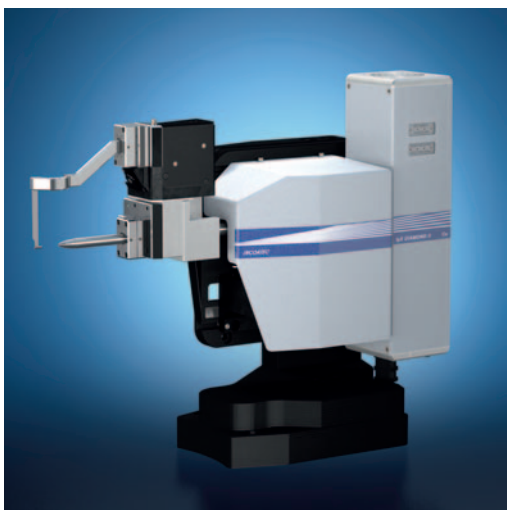
Indium: short but sweet

Our high-brilliance METALJET can also be configured to provide an extremely intense indium X-ray beam, the shortest wavelength available in the home laboratory. Indium is thus ideal for advanced applications including high pressure and charge density.

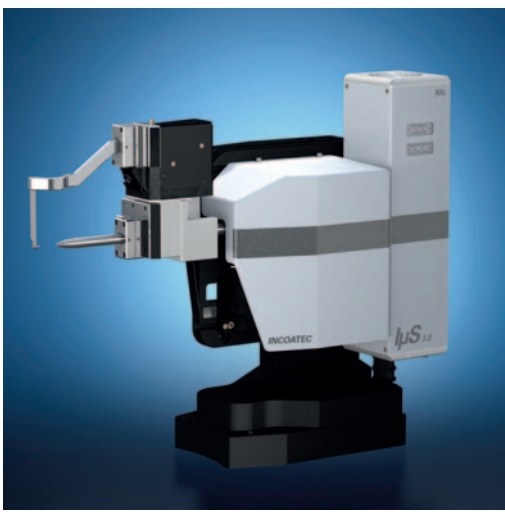
Liquid metal METALJET source with In or Ga radiation



IμS DIAMOND II X-ray source with Ag, Mo or Cu radiation



IμS 3.0 X-ray source with Ag, Mo or Cu radiation



IμS 3.0: Top performance by design

Bruker and Incoatec pioneered the first modern microfocus sources. More than 1,700 of these outstanding sources are in the field and have established an unequalled record for performance and reliability. Other microfocus sources still use tubes designed for radiography or Non-Destructive Testing (NDT).

The IμS 3.0 features the first tube which was designed and manufactured by Incoatec exclusively for crystallography. These unique tubes feature optimized take-off angles and electron optics to achieve up to four times the intensity of competing sources based on NDT tubes.

IμS DIAMOND II: Rotating anode performance with sealed tube convenience

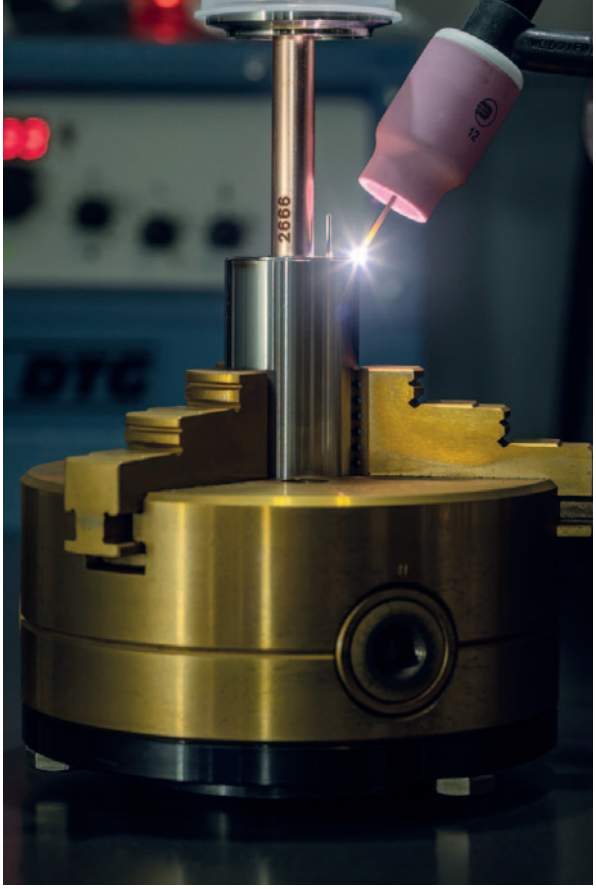
Isotopically pure diamond conducts heat better than any other known material, making it perfect for cooling the intense heat loads in a modern microfocus source. Incoatec has implemented this technology in the diamond hybrid anode. To take full advantage of this technology, the IμS DIAMOND II features a newly developed cathode to advance the electron beam properties, and active electron lenses allowing fast ramp-up and ramp-down as well as instantaneous wavelength switching in dual wavelength systems. The further increased power load on the anode leads to X-ray intensities that outperform conventional microfocus rotating anode generators.

The IμS – Simply Brilliant

The IμS 3.0 and the IμS DIAMOND II both set new standards with respect to brightness, stability, and ease of use for all applications. Eliminating any compromise in the design allows us to deliver the best-ever IμS technology for your most challenging experiments. The IμS 3.0 and the IμS DIAMOND II of course deliver the same unique all-air-cooled operation and the same legendary reliability you have come to expect.

METALJET D2 PLUS: Beamline intensities in your home lab

Bruker collaborated closely with Excillum during the development of the METALJET source, and with over ten years of operational experience, Bruker has a deep understanding of the technology and offers by far the most advanced, sophisticated and reliable METALJET-based solutions. In the D8 VENTURE, the METALJET is seamlessly integrated. By constantly monitoring all aspects of the source operation, our sophisticated firmware ensures ultra-stable long-term performance. Finally, while the relatively high-figure error of other multilayer optics typically leads to a loss of brilliance of up to 70%, our unique, patented low-figure error HELIOS optics were specifically developed and optimized for the METALJET and are the only optics that fully preserve the inherent brilliance of this exciting X-ray source.



An entire tube production line – for the best IµS sources

All IµS tubes are designed, developed and manufactured exclusively by Incoatec. Indeed, Incoatec is the only company that makes microfocus tubes optimized for X-ray diffraction. These optimized tubes offer higher performance and higher quality, resulting in longer tube lifetimes.

Our X-rays are "Green"

Future-Proof Solutions

With the D8 QUEST and D8 VENTURE, we are following design principles that protect the environment. Our PHOTON III detector and advanced IµS DIAMOND II and METALJET D2 PLUS sources consume very little energy and do not need water cooling.

This significantly reduces carbon emissions and water consumption, improves reliability, and reduces the cost of ownership.

Saves 26 t of CO_2 per year *

No Water Supply

- Air-cooled PHOTON III
- Air-cooled IµS DIAMOND II microfocus source
- METALJET D2 PLUS, no external cooling water required

Saves 1,700 m^3 cooling water per year *

Single-Phase Power

- Ultra-low power consumption of all PHOTON III detectors
- IµS DIAMOND II uses 99% less energy than conventional rotating anodes
- METALJET D2 PLUS delivers beam intensities more than three times higher than microfocus rotating anodes, using only a fraction of a rotating anode's power consumption
- Single-phase power and standard circuit breaker for ease of installation

Saves 43,000 kWh electrical energy per year *

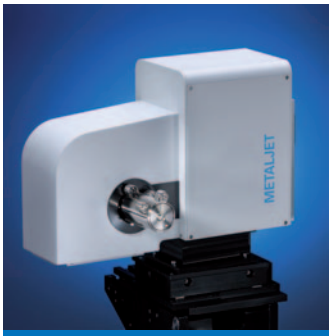
*) 24 hours, 300 days with IµS DIAMOND II and PHOTON III

IμS 3.0 with HELIOS MX for Cu, Mo and Ag radiation

- The IμS 3.0 microfocus source excels with low maintenance and high reliability
- Up to twice the intensity of conventional micro-focus sources
- First-ever microfocus source specifically designed and optimized for X-ray diffraction
- Third-generation optics with best spectral purity, excellent reflectivity, and a near-zero X-ray background
- Three-year source warranty

IμS DIAMOND II for Cu, Mo and Ag radiation

- The average intensity is 20% higher than that of a microfocus rotating anode source
- The best optics put all the X-rays on the sample for up to 10 times lower scattered X-ray back-ground
- Unique 99% uptime guarantee
- 10 times better stability than rotating anodes – for the best data quality
- Newly developed cathode for advanced electron beam properties
- Active electron lenses for fast ramp-up and ramp-down
- Instantaneous wave-length switching in dual wavelength systems



METALJET with HELIOS MX for Ga and In radia-tion

- The METALJET uses a liquid target consisting of gallium or indium rich alloys
- Compared to Cu radiation Ga Kα radiation allows higher multiplicity data sets in less time
- In Kα radiation is a superb alternative to Ag Kα for high pressure and charge-density studies
- Fresh, self-healing target for high power load with long-term constant beam intensity

Source	Typical tube lifetime [years]	Relative intensity [X-rays / mm^2 -sec]
Bruker IμS 3.0 Cu	**5**	**8×10^{10}**
Conventional microfocus source Cu	3	2×10^{10}
Bruker IμS 3.0 Mo	**5**	**3.1×10^{9}**
Conventional microfocus source Mo	3	1×10^{9}
Bruker IμS DIAMOND II Cu	**5**	**1.6×10^{11}**
Conventional rotating anode Cu	1	1.6×10^{11}
Bruker IμS DIAMOND II Mo	**5**	**9.5×10^{9}**
Conventional rotating anode Mo	1	5.4×10^{9}

Made to perform

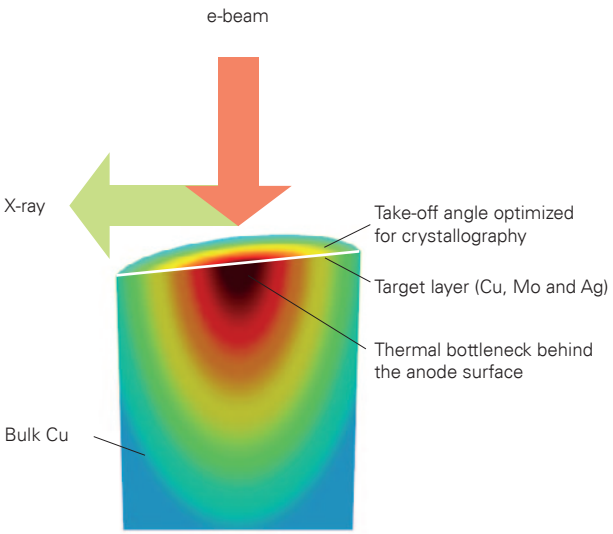
Higher intensities are achieved in the IμS 3.0 and IμS DIAMOND II by optimizing all the critical tube parts, such as the cathode, electron optics and take-off angles.

In addition, the diamond hybrid anode used in the IμS DIAMOND II features an isotopically pure diamond substrate that is coated with a layer of the target material taking advantage of the ultimate thermal conductivity of the isotopically pure diamond to achieve even higher intensities. An active electron lens allows fast ramp-up and ramp-down. Combined with the advanced electron beam provided by the newly developed cathode the IμS DIAMOND II delivers an intensity that outperforms conventional microfocus rotating anodes.

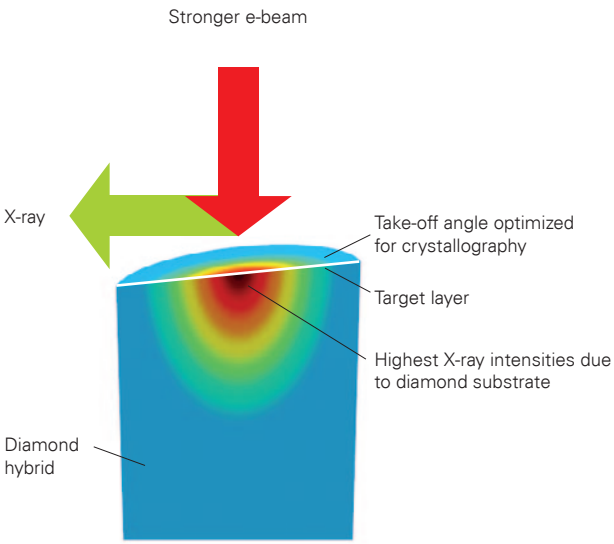
The high-brightness cathode provides the most homogeneous electron beam with the highest intensity of any microfocus tube.

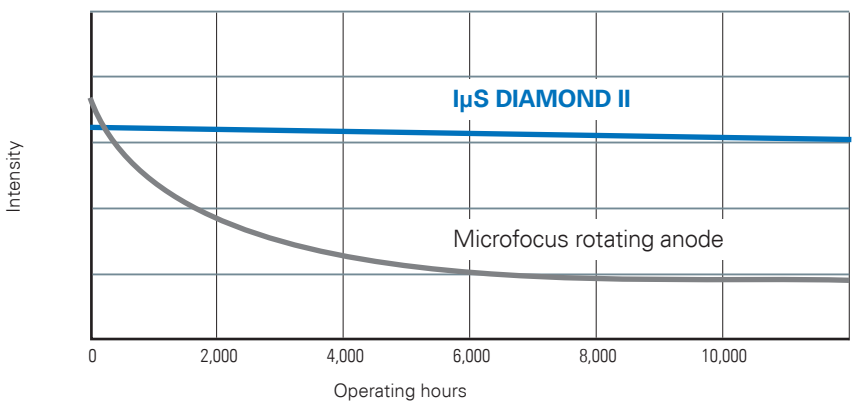
Rotating anodes typically suffer rapid degradation of output due to the repeated heating-cooling cycles of the anode's surface, leading to surface microcracking of the anode. In contrast, the heat load on the IμS DIAMOND II surface is constant over time, making the output of the IμS DIAMOND II much more stable. The IμS DIAMOND II source also outperforms microfocus rotating anodes without the headache of high running costs and without routine maintenance.

IμS 3.0
Cu/Mo/Ag anode



IμS DIAMOND II
hybrid anode, Cu/Mo/Ag





D8 QUEST

- Small footprint without sacrificing experimental flexibility
- Accommodates single-source configurations
- Exterior dimensions: 187 cm × 130 cm × 114 cm (h × w × d)

Configuration example:
- IμS 3.0 sealed source, Mo
- HELIOS optics
- FIXED-CHI goniometer
- PHOTON III detector

D8 QUEST and D8 VENTURE: Systems as individual as your research

We are proud to present the second generation of our D8 Crystallography Solutions.

With our D8 Crystallography Solutions, we offer a pioneering diffractometer concept with flexibility and modularity. The D8 QUEST and the D8 VENTURE can be perfectly configured for the demands of any imaginable application in single crystal X-ray diffraction.

Just follow three simple steps:

1. Choose your preferred wavelength from a wide variety of X-ray sources and optics.
2. Combine your preferred source with the goniometer and enclosure of your choice.
3. Add the state-of-the-art photon-counting PHOTON III detector with an active area fitting your needs…

   …and you are ready to run the most sophisticated analytical experiments. Do you need two wavelengths at your fingertips? Dual-source configurations are also readily available with our D8 Crystallography Solutions and, in addition, a single-source instrument is upgradable to a dual-source configuration at any time.

Real-time status information about the configuration and components are carefully logged and conveniently stored with all other experimental settings, ready to use for automated reports and publications.

D8 QUEST and D8 VENTURE are both built for excellent sample access and sample visibility. Their absolutely open design protects your investment with maximum flexibility for future extensions.

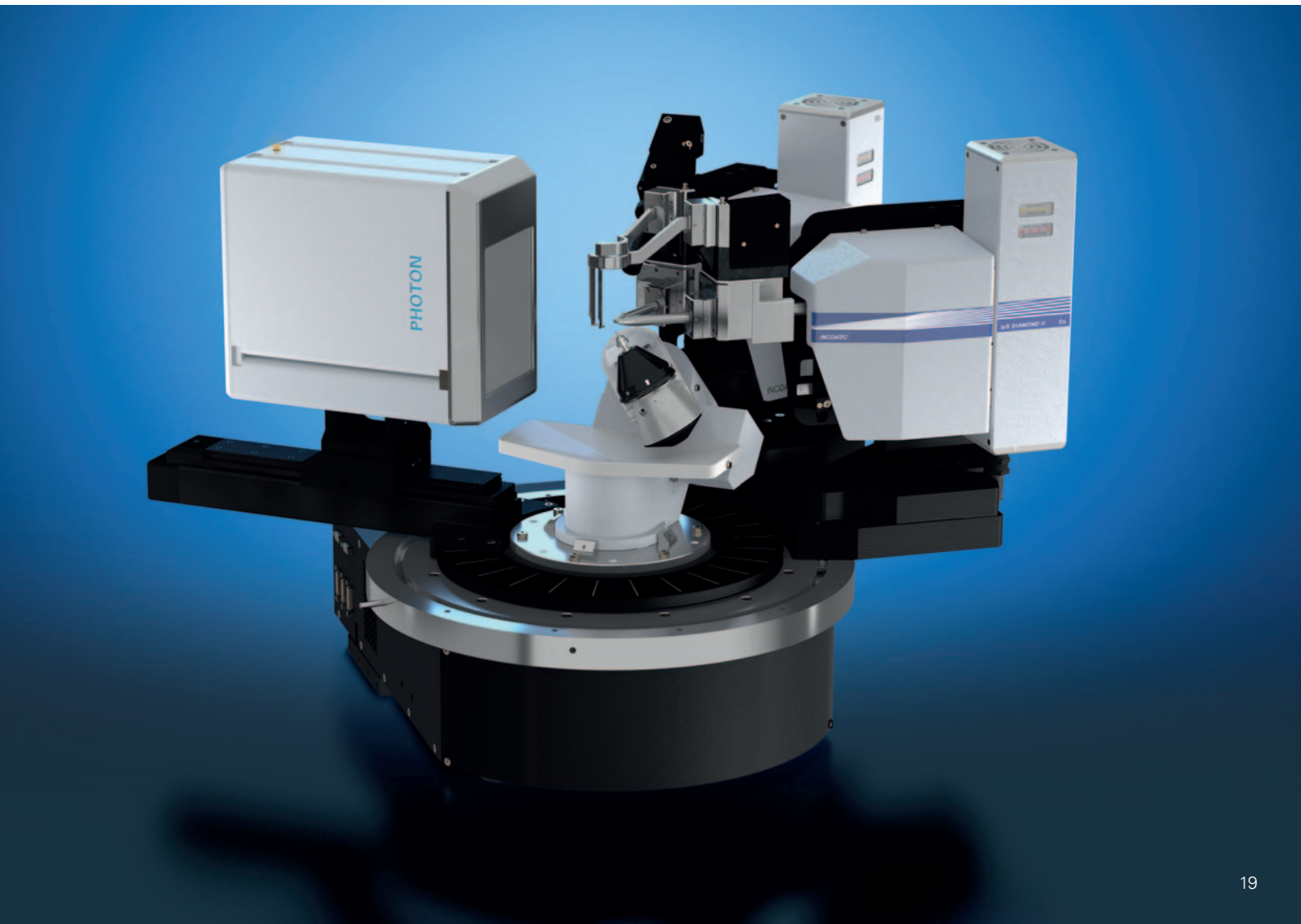
Make your choice and get the best possible structure from your sample – guaranteed!

D8 VENTURE

- More room for dual-source setups
- Accommodates single- and dual-source configurations
- Exterior dimensions: 202 cm × 168 cm × 129 cm (h × w × d)

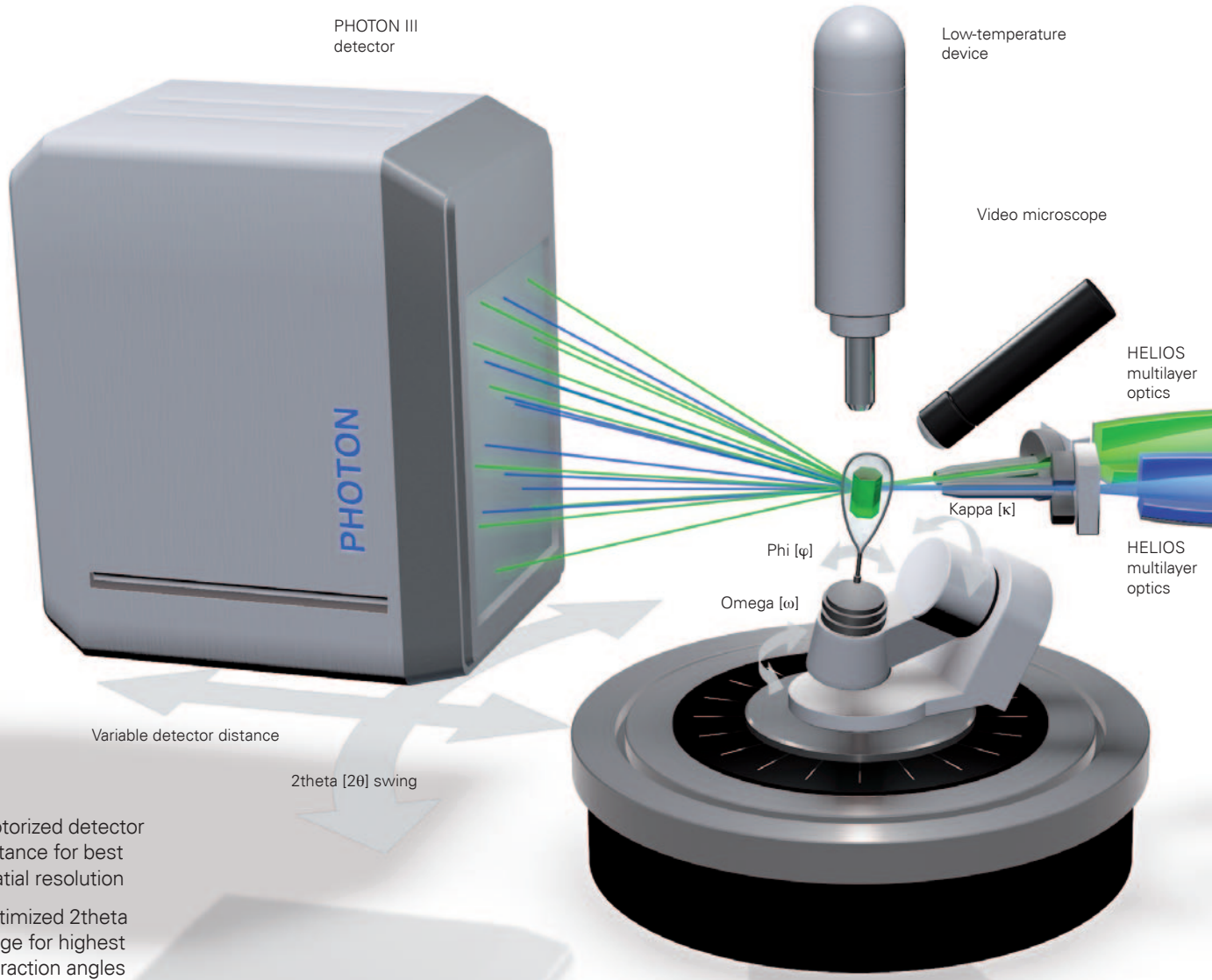
Configuration example:
- IμS 3.0 sealed source, Mo
- IμS DIAMOND II, Cu
- HELIOS optics
- KAPPA goniometer
- PHOTON III detector


PHOTON
INCOATEC
IμS 3.0
Mo


PHOTON

Love FIXED-CHI? Prefer KAPPA? We invented them both!

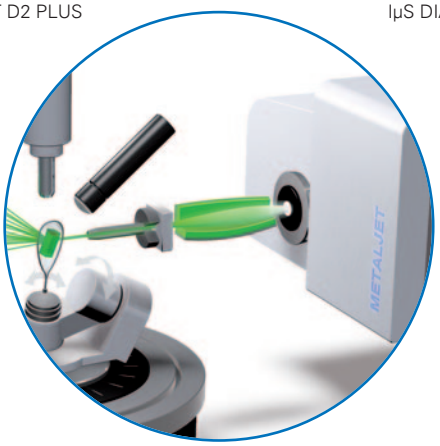
- Large active-area PHOTON III detector
- Active area size: 70, 140 and 280 mm^2, gap-free



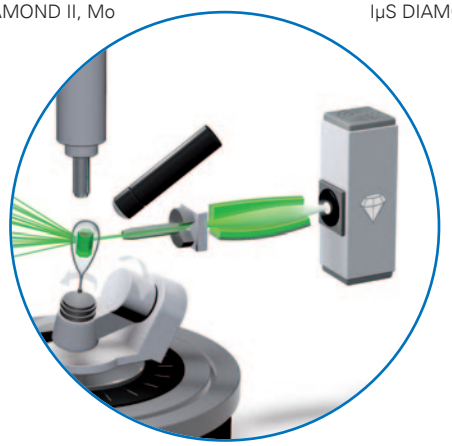
- Motorized detector distance for best spatial resolution
- Optimized 2theta range for highest diffraction angles

- KAPPA goniometer for greatest flexibility
- Smallest sphere of confusion

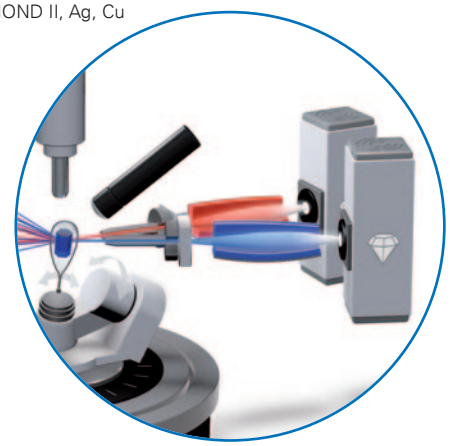
Single-source geometry with
METALJET D2 PLUS



Single-source geometry with
IμS DIAMOND II, Mo



Dual-source geometry with
IμS DIAMOND II, Ag, Cu



Mo IμS DIAMOND II,
microfocus tube

Cu IμS DIAMOND II,
microfocus tube

- Single- and dual-source configurations for high versatility
- KAPPA goniometer for greatest flexibility
- FIXED-CHI goniometer for simplicity
- Sphere of confusion (SOC) < 7 micrometers
- Best scaling for strongly-absorbing samples
- Constant sample scattering volume in the beam
- Highest intensity from microcrystals

Whatever your goniometer of choice – three-axis FIXED-CHI or four-axis KAPPA – optical encoders ensure extremely high angular precision, and fast goniometer positioning enhances productivity no matter what the focus of your applications. What would a high-precision goniometer be without easy crystal mounting and constant sample monitoring? D8 QUEST and D8 VENTURE make sample alignment a real pleasure: large doors give you excellent access to the goniometer. Dimmable LED sample illumination greatly enhances the crystal image quality. The crystal image is captured by a high-resolution video microscope, and the video stream can be viewed remotely during the entire experiment.

The new beam path was designed for easiest down-stream alignment and maximizes the accessible 2theta range for high-resolution work. This is an important asset for your charge-density studies or data sets with copper radiation that require high-2theta data.

Smallest sphere of confusion (SOC)

Our D8 goniometer is designed for the highest accuracy and precision, superb alignment, and long-term reliability. Our goniometer has the smallest error in intersection of the instrument axes, provides the best sphere of confusion (SOC), and is unsurpassed by any other goniometer. Even the tiniest microcrystal stays reliably centered during the entire data acquisition, guaranteeing the best possible structure.

Best Hardware
+ Best Software
= Best Structure

The best structures start with APEX4

Software is a crucial part of the investment in a crystallographic system.

With the new APEX4 suite, Bruker continues its long history of offering the most advanced software package for structure determination, from convenient sample centering to stunning results to publication-ready reports.

- APEX4 is intuitive, easy to learn and to use.
- APEX4 uses world-class algorithms and scientific engines to handle crystallographic challenges including twinning, disorder and modulated structures.
- APEX4 offers a user-selectable level of automation. This allows novice users to quickly learn, while experienced crystallographers can take complete control.
- APEX4 integrates the power of STRUCTURE finder.

APEX4 – usability and performance without compromise

For good reason, the majority of chemists, crystallographers, and mineralogists around the world rely on our software to tackle their most difficult crystallographic challenges.

And mow, the world's most powerful crystallographic software package is also the easiest to learn and use.

We're constantly working with our customers, listening, learning, and incorporating all that knowledge to improve our software.

The new APEX4 software suite incorporates all the experience and knowledge gained from our customers' experience to improve every aspect of the user experience: from a new, more flexible and more intuitive user interface to the most powerful analytical engines.

A perfect fit for everybody

You can select your preferred level of automation – depending on the crystallographic challenge you are facing, always tuning the package to your highest convenience.

Novice user, fully automated operation

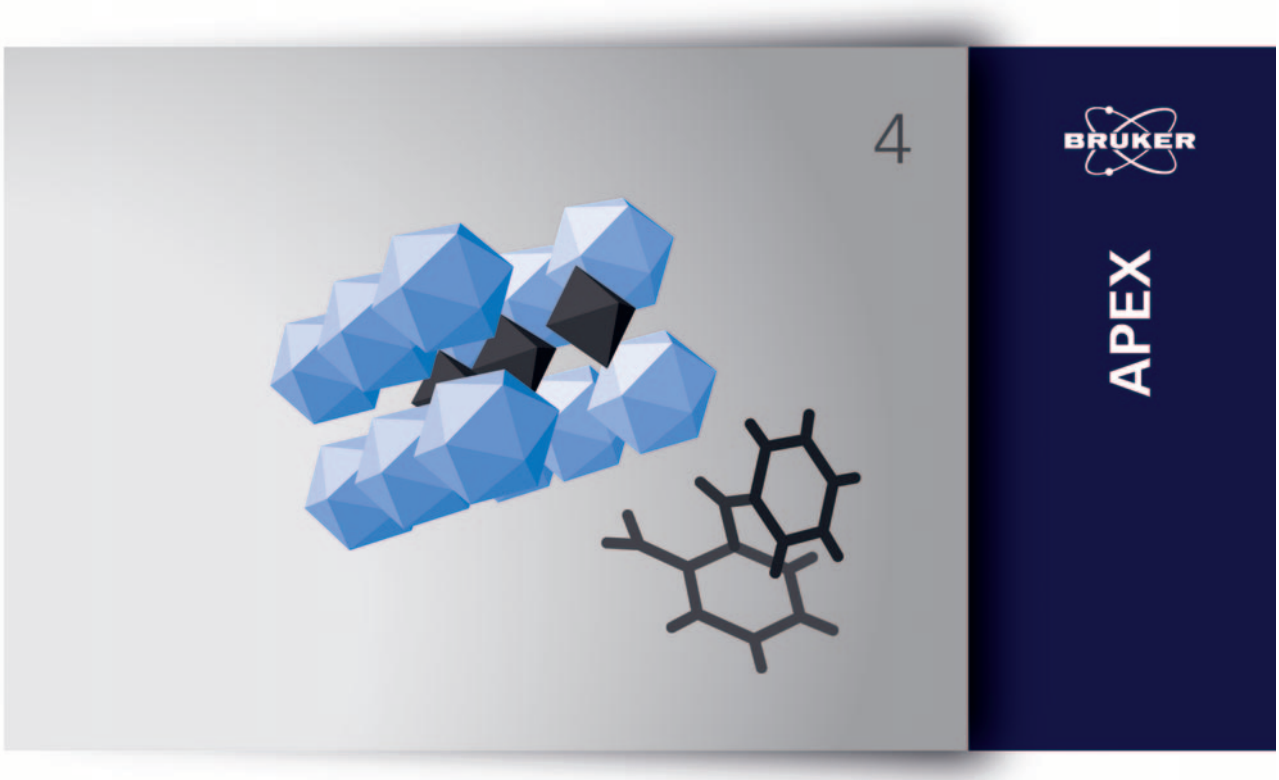
- User only mounts and enters elements
- "Centering" to "Report" is done automatically by APEX4
- No further user intervention required
- Throughout APEX4 "green-yellow-red" backgrounds guide novices to the perfect structure and provide a quick overview to experienced crystallographers

Regular user, semi-automated operation

- Available for all main plugins
- Full control over parameters
- Automated "Finish" available at any time

Expert user, manual operation

- Step-by-step operation
- Full control over parameters
- Expert functionality



APEX4 user benefits

- APEX4 offers a range of new features and capabilities making it both more powerful and also easier to use
- New GUI with selectable automation, easier to learn and use for novices but offering full control for the expert
- Simplified & Automated Twin handling
- GPU implementation of RLATT for faster processing and improved feedback
- Integrated Database check for CSD, COD and local structures
- Greatly improved video quality – the best images for today's ever-smaller crystals
- One-button installer with auto-update function

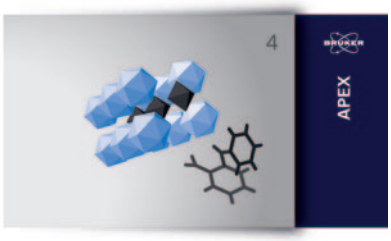
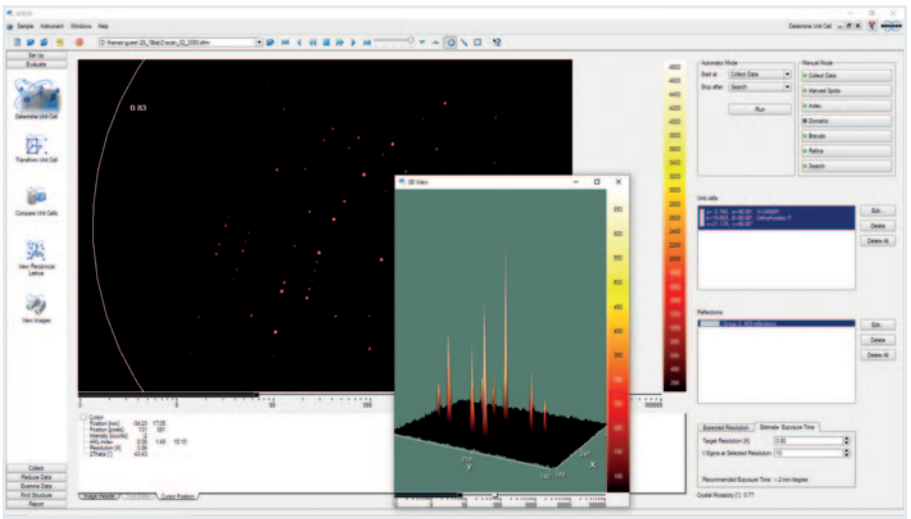


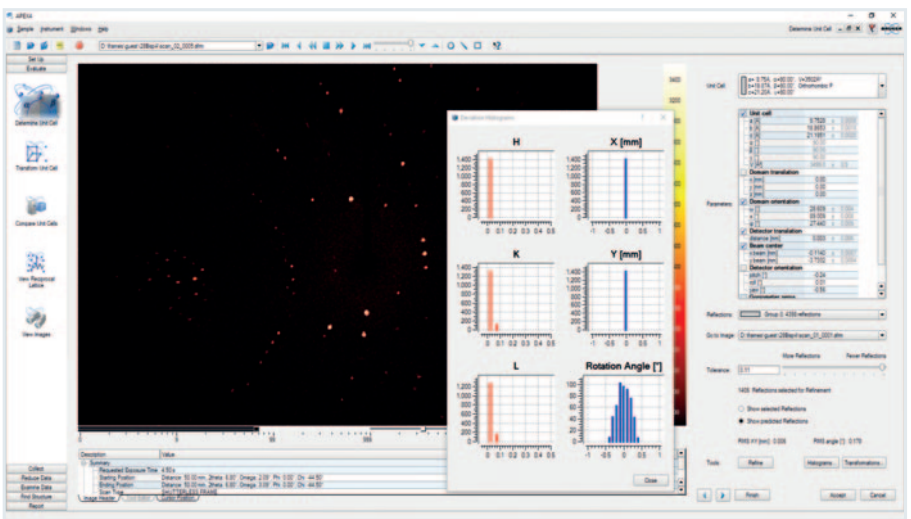
Image Analysis

The intuitive APEX4 diffraction image interface provides all the means for image analysis, including zooming and panning, 3-D views, line graphs, rocking curves, resolution rings, and many more. These tools make judging data quality or investigating crystallographic challenges easy and efficient.



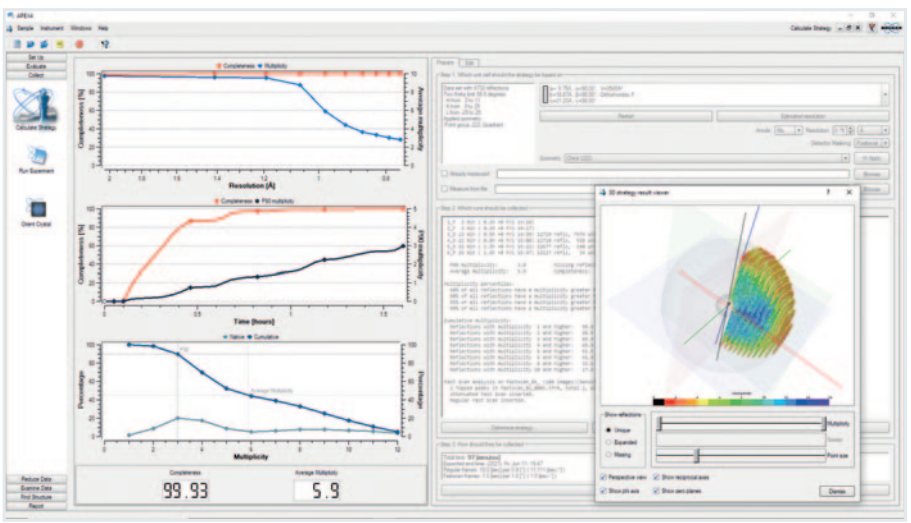
Unit Cell Determination

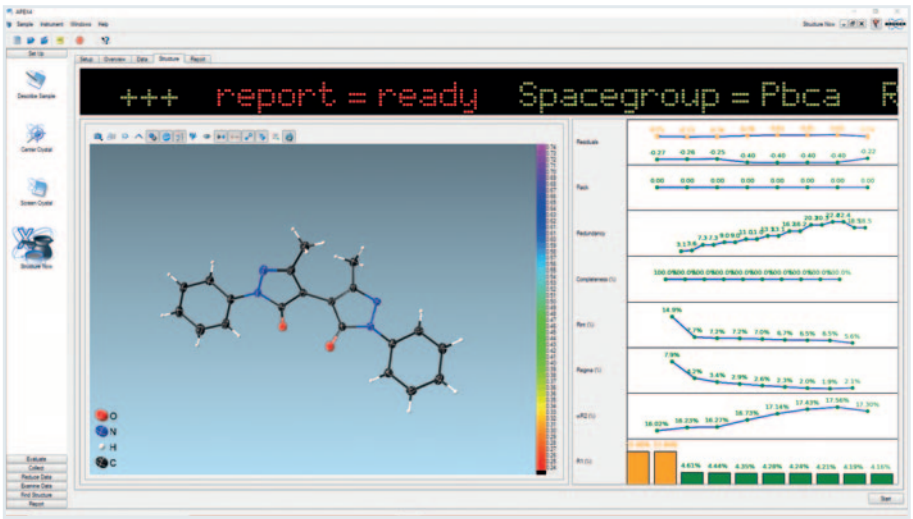
Our unique combination of Fast Fourier, Difference Vector and Least Squares techniques ensures reliable indexing of the most difficult data. Full nonlinear least squares cell refinement with graphical feedback, diffraction spot overlay, Bravais lattice determination, and tools for matrix manipulation complete this module.



Data Collection Strategy Planning

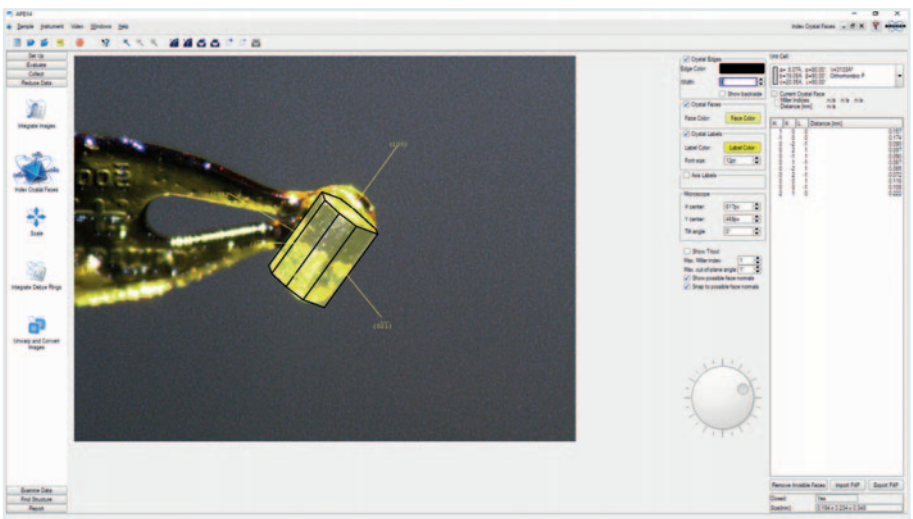
Make the most of your instrument time and collect complete data fast and efficiently. The APEX4 suite ensures highest possible completeness and optimized instrument usage. Confidently rely on an automated strategy determination that lets you adjust parameters and lets you be in the driver's seat.





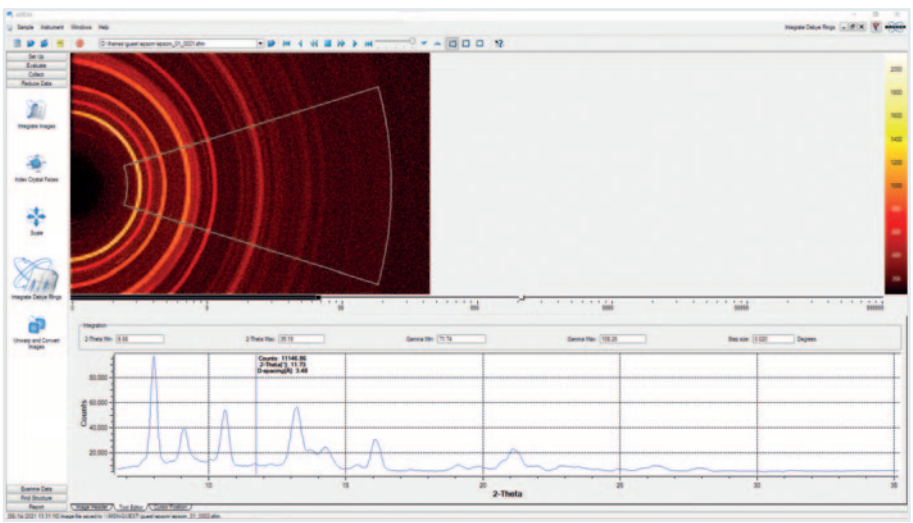
Automated Structure Determination

STRUCTURE NOW combines intelligent, decision-making algorithms with machine reasoning that lets the software learn how to best collect and process data. Just specify the formula, and let STRUCTURE NOW do the rest. The module will automatically determine and refine the structure, provide molecular graphics and a complete HTML report – in short: everything needed for a successful publication.



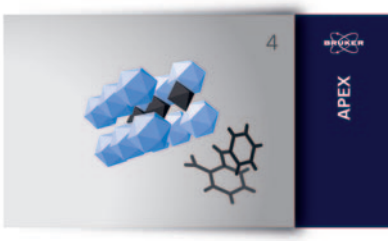
Face Indexing

Crystal description for numerical absorption correction is only a few mouse clicks away. Easily and intuitively describe a crystal's shape from a prerecorded movie with easy-to-use tools and intelligent helpers.



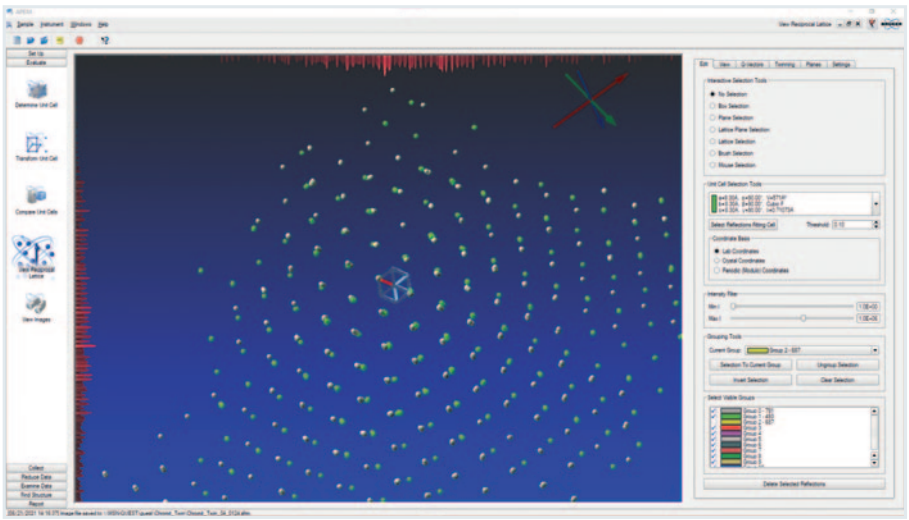
Powder Diffraction

It doesn't always have to be a single crystal. Your single crystal diffraction system is perfectly suited for collecting and processing high-quality powder diffraction data. The plug-in handles diffraction from polymers, fibers, and partially-oriented powders and provides export to the full suite of Bruker XRD software.



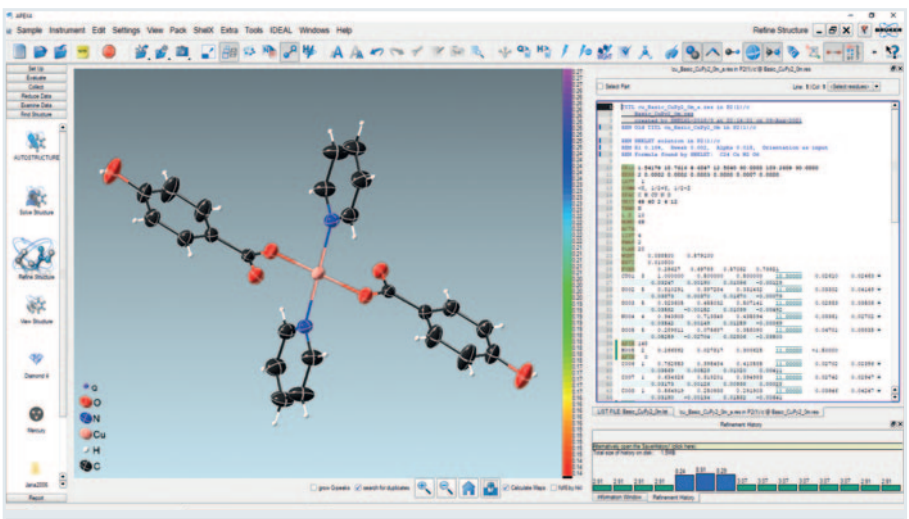
Reciprocal Lattice Viewer

The GPU accelerated plug-in – faster and without an upper data limit – helps to display and interactively modify reflection arrays. Visually separating twin components and determining q vectors of incommensurate structures are now faster than ever with many new options. Without a doubt, the reciprocal lattice viewer is one of the most powerful tools for tackling challenging crystallographic problems.



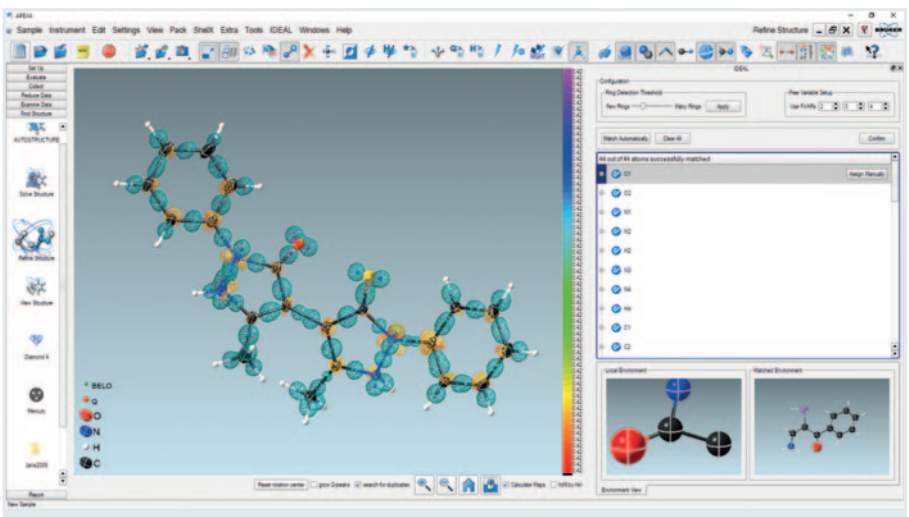
Model Building

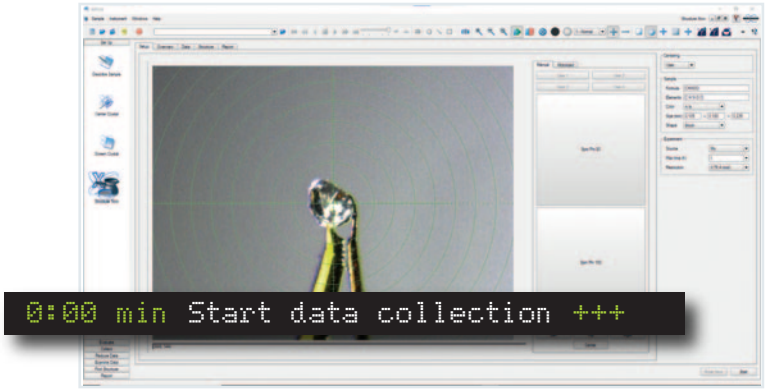
A modern approach to interactive model-building for structure refinement is powered by SHELXLE. A creative combination of graphical interface and text-based input with auto-completion makes structure refinement easy. Electron density maps let you look beyond the spherical model and let you capture minute details of your structure.

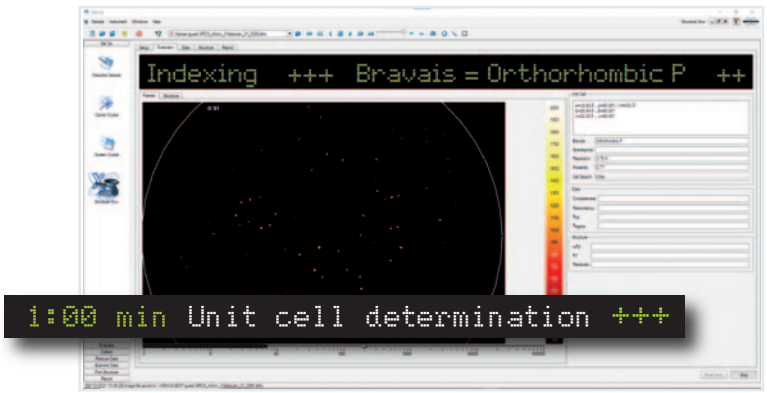


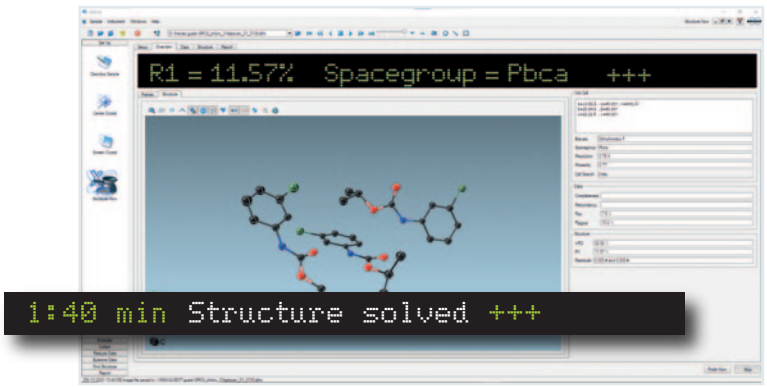
Refinement Beyond the IAM

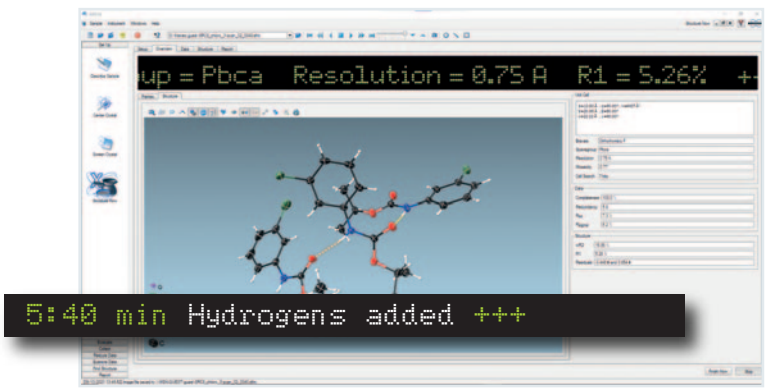
IDEAL goes beyond the traditional Independent Atom Model (IAM), adding scattering contributions of bonds and lone pairs to improve the quality of the model. With IDEAL, it is finally possible to combine crystallographic and quantum chemical treatment of the organic solid state.

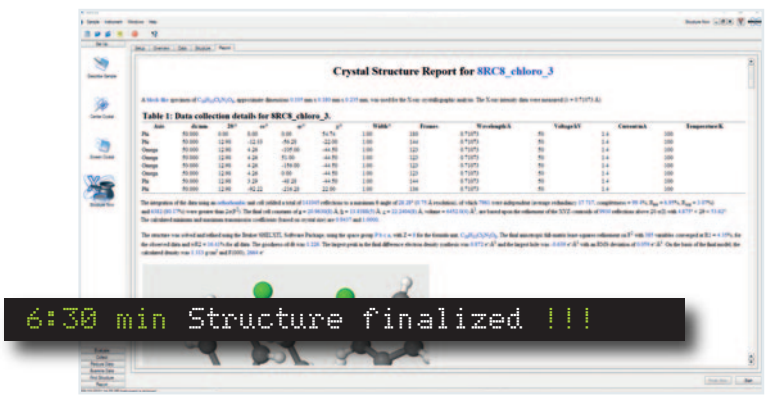












Structure now

AI technology drives better automation

Bruker was the first to introduce a fully automated structure determination routine in APEX3. Now in APEX4 our new automation plugin, STRUCTURE NOW, applies the latest Artificial Intelligence (AI) technology to better automate tasks for the user. Automating processes saves the user time and energy, makes their job simpler, allowing them to work more efficiently and productively.

Combining machine learning and reasoning

STRUCTURE NOW combines intelligent, decision-making algorithms and introduces machine learning that lets the software learn how to best collect and process data. APEX4 can improve data quality and crystal structures automatically and autonomously.

Automation or manual control – your choice

AI is an extremely powerful new tool for science but there are of course still tasks that demand the experience and expertise of the crystallographer. STRUCTURE NOW thus gives you the choice to use smart automation when you want it and keep manual control when you need it. With the most comprehensive collection of crystallographic tools, our expert users tackle the most challenging samples easily and efficiently.

Overview of Features and Benefits

	Feature		Benefit
PHOTON III Detector	Photon-counting pixel-array detector	5th generation pixel array detector technology	Higher speed and sensitivity, best data quality
	Large active area	100 × 70 mm^2 100 × 140 mm^2 200 × 140 mm^2	Faster data collection
	Fast readout time	14 msec	
	Very high count rate	Up to 4 × 10^6 counts/pixel-sec	
	Readout dead time	0 sec (full shutterless operation)	
	No dead areas	Single, monolithic silicon sensor	Improved data quality
	High dynamic range	> 200,000	
	No charge sharing noise	0 electrons charge-sharing noise	
	Very low parallax	< 1 pixel (for Cu, Ga, Mo, Ag, In)	
	No count-rate nonlinearity	< 1% nonlinearity up to full count rate	
	High detective quantum efficiency (DQE)	> 90% Ga to In	
	No operating gas or cooling water	Completely sealed design, air-cooled	No maintenance, high uptime
	High reliability	Warrantied for 3 years	
IμS 3.0 Source	High intensity beam, completely air-cooled	Cu, Mo, Ag radiation	High performance, ultra-low maintenance, optional dual-wavelength configuration
IμS DIAMOND II Source	Very high intensity beam, completly air-cooled, revolutionary e-beam and cooling technology	Cu, Mo, Ag radiation	Rotating performance from a microfocus sealed tube, ultra-low maintenance, optional dual-wave-length configuration
METALJET D2 PLUS Source	Highest intensity beam	Ga, In radiation	Ultimate performance for small, weakly diffracting samples
D8 Goniometer	Very low sphere of confusion	< 7 μm	Best data quality
	High speed	Up to 1,200 deg/min (omega)	Faster data collection
	Fixed chi geometry		Economical, general purpose
	Kappa geometry		Highest flexibility
APEX4 Software	Most comprehensive software package for single crystal X-ray diffraction (SC-XRD) using well-tested first-class algorithms		
	User-selectable level of automation: easy to learn for novices, complete control for experienced crystallographers		
	State-of-the-art responsiveness: incorporating user feedback from hundreds of installations		
	Unparalled twin handling: the most powerful reciprocal lattice viewer to tackle all crystallographic problems		
	STRUCTURE NOW: first automation layer applying artificial intelligence		
	Model Building: first class interactive model-building and refinement powered by SHELXLE		

aim 03044

Bruker AXS
info.baxs@bruker.com

Worldwide offices
bruker.com/baxs-offices

Online information
bruker.com/scd

bruker.com