SINGLE CRYSTAL X-RAY DIFFRACTION

D8 QUEST ECO

Crystal Structures for Chemical Research and Education

Innovation with Integrity

D8 QUEST ECO
Crystallography has never been easier

Driving modern science

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

As the frontiers of science advance, the need for chemical structures is growing more acute as seen in the wider use of crystallographic instruments — with more power, higher speed and improved ease of use.

Crystal structures accessible to all

Our driving passion is to provide scientists with the best tools for crystallography.

Building on decades of experience in creating top-quality instruments, Bruker has re-imagined X-ray crystallography in a compact, cost-efficient platform.

The D8 QUEST ECO features robust, straight-forward operation. The easy-to-learn APEX4 software interface guides chemists through the entire experiment from collecting the best data to accurately solving the crystal structure. APEX4 includes the STRUCTURE NOW program, for the option of fully automated structure determination.

Ready to go

The D8 QUEST ECO includes everything you need to solve crystal structures and can be installed with no special requirements.

Chemistry

Geosciences

Pharmaceutical

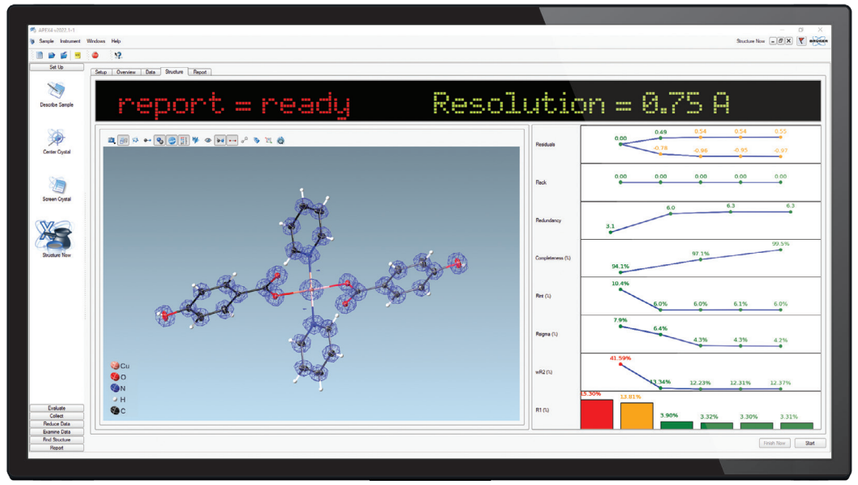
Materials

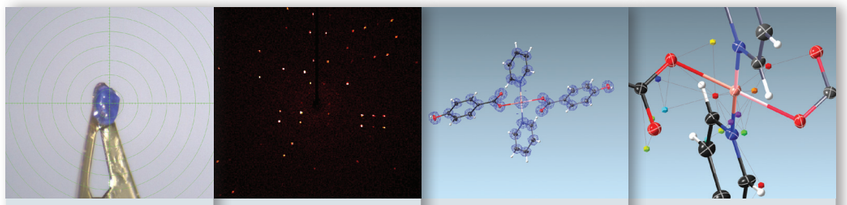
Education

Automatic STRUCTURE determination is NOW

STRUCTURE NOW is the first and only program that enables chemists to routinely determine 3D atomic structures without extensive crystallographic training.

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





Characterize crystal

Accurately center and quickly characterize your crystal

- Diffraction quality
- Unit cell and Bravais type
- Search databases

Collect data

Automatically calculate the best strategy for any crystal

- Complete high-quality data
- Large unit cells
- Low symmetry
- Twinned crystals

Determine structure

Diffraction data are processed and an electron density map calculated. Atoms and connectivity are modelled into the density map

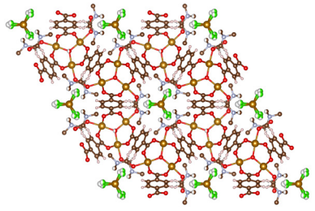
- Structure refinement
- Model quality indicators

Analyze structure

The structure helps to understand the chemistry

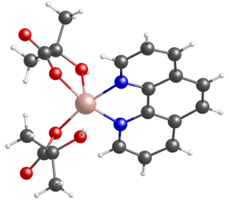
- Highly accurate model
- Electron density maps reveal minute details
- Generate report — experimental details, structure, and quality indicators

D8 QUEST ECO for research
Unambiguous chemical structure



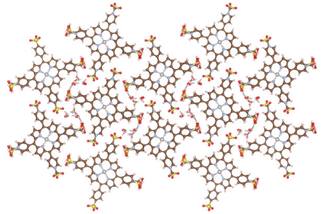
Synthetic chemistry

Many molecules essential to modern life need to be synthesized in the laboratory and designed for specific functions. The precise connectivity of atoms and their orientation in three dimensions dictates these functions. Crystallography is the only method that unambiguously determines the absolute structure of molecules and is therefore key to successful synthetic chemistry.



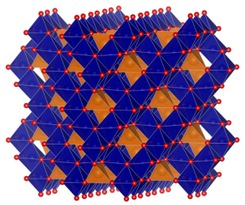
Inorganic chemistry

The broad scope of research in inorganic chemistry produces a huge variety of new reaction products. Crystallography is a fast and convenient method to confirm atomic composition, connectivity and configuration of these compounds. Inorganic chemistry departments around the world take advantage of the versatility of crystallography to drive research across the entire field.



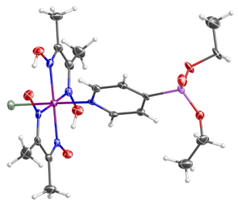
Materials sciences

Modern society increasingly demands new materials to drive development in a sustainable manner. New energy storage materials, reducing air pollution, water conservation, new electronics devices – all of these fields rely on a detailed structural understanding of the underlying chemistry.



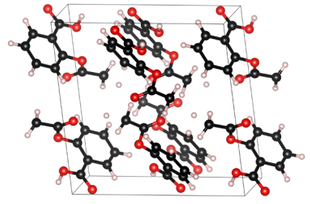
Geological sciences

With just a few exceptions, minerals are natural occurring crystals and the geological world is mostly a crystalline world. Crystallography is widely used to quickly and accurately characterize the mineral components of geological samples. Knowing the chemical structure of minerals helps geochemists to understand their role in large-scale geological processes and sheds new light on the sustainable use of natural resources.



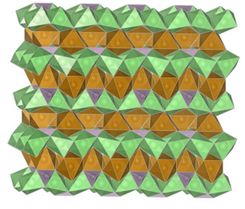
Industrial chemistry

Whether you work in specialty chemicals, energy, plastics, agrochemicals, or any other segment, the industry is getting more complex, increasing the drive for the development of more advanced chemicals. 3D-structures determined by crystallography are essential for polymorph analysis, catalysis research, and increasingly in the development of sustainable polymers.



Pharmaceutical sciences

Research into new active pharmaceutical ingredients or development of solid-state formulations are both reliant for success on the answers crystallography provides. Absolute configuration is essential to the development and certification of new active pharmaceutical ingredients. Crystallography further provides a complete description of unit cell packing required for optimizing the solid-form drug. Additionally, crystallography provides a high-resolution complement to routine powder X-ray diffraction.



Energy storage and battery research

Metal-ion batteries are key enablers in today's transition from fossil fuels to renewable energy with ingeniously designed materials being the technology driver. Crystallography plays a crucial role in understanding how to wisely manipulate atoms to build attractive structural frame-works of better electrodes and electrolytes for the next generation of batteries.

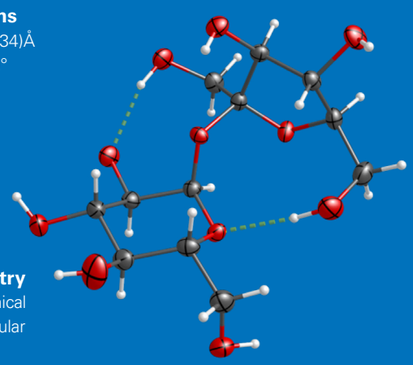
Seeing is believing

Humans are highly visual, and the ability to directly see and examine our subject in three dimensions gives us powerful insight into the structure and chemistry of molecules and solid-state materials. Crystallography is a powerful addition to the lab as no other analytical method provides direct determination of 3D structures at atomic resolution with such accuracy and precision.

Highly accurate positions
- Bond length, 1.4231 (0.0034)Å
- Bond angles, 111.10 (0.22)°

Unit cell parameters
- Fast database check
- Rapid phase identification by powder XRD

Absolute stereochemistry
- Unambiguous stereochemical description of chiral molecular entities



Structural details
- Static disorder
- Thermal disorder
- Charge density

Composition
- Atom types
- Occupancies
- Mixed sites

3D arrangement
- Hydrogen bonding
- Intermolecular bonding
- Solvent
- Crystal packing

D8 QUEST ECO crystallography for all
Accessible crystal structure analysis

The D8 QUEST ECO is the affordable solution packed with features to make crystal structure analysis accessible to more researchers in more laboratories.

Simple to use for non-specialists and students

Mount your crystal, close the safety door and you are ready to measure. The easy-to-follow APEX5 workflow guides non-specialists through data collection, processing, and structure determination. Extensive graphical feedback helps students develop a strong understanding of the technique.

For ultimate convenience STRUCTURE NOW will automatically determine the structure for you.

The ideal addition to the busy X-ray lab

Is your current X-ray instrument permanently overbooked? Then the D8 QUEST ECO is a cost-effective support instrument to ease the burden. Add a D8 QUEST ECO to your lab and free-up time on your existing system for the really challenging crystals.

Don’t compromise your research

The full 3-axis goniometer equipped with a state-of-the-art PHOTON III detector enables you to collect publication-quality atomic-resolution data from the widest variety of crystals. APEX5 provides all the tools required for advanced experiments to get the best structures from more complex datasets.

Install in any lab

The compact system fits into even the smallest laboratories, and requires nothing more than standard, single-phase electricity supply. The fail-safe radiation enclosure means the system is perfectly safe for researchers and students alike.

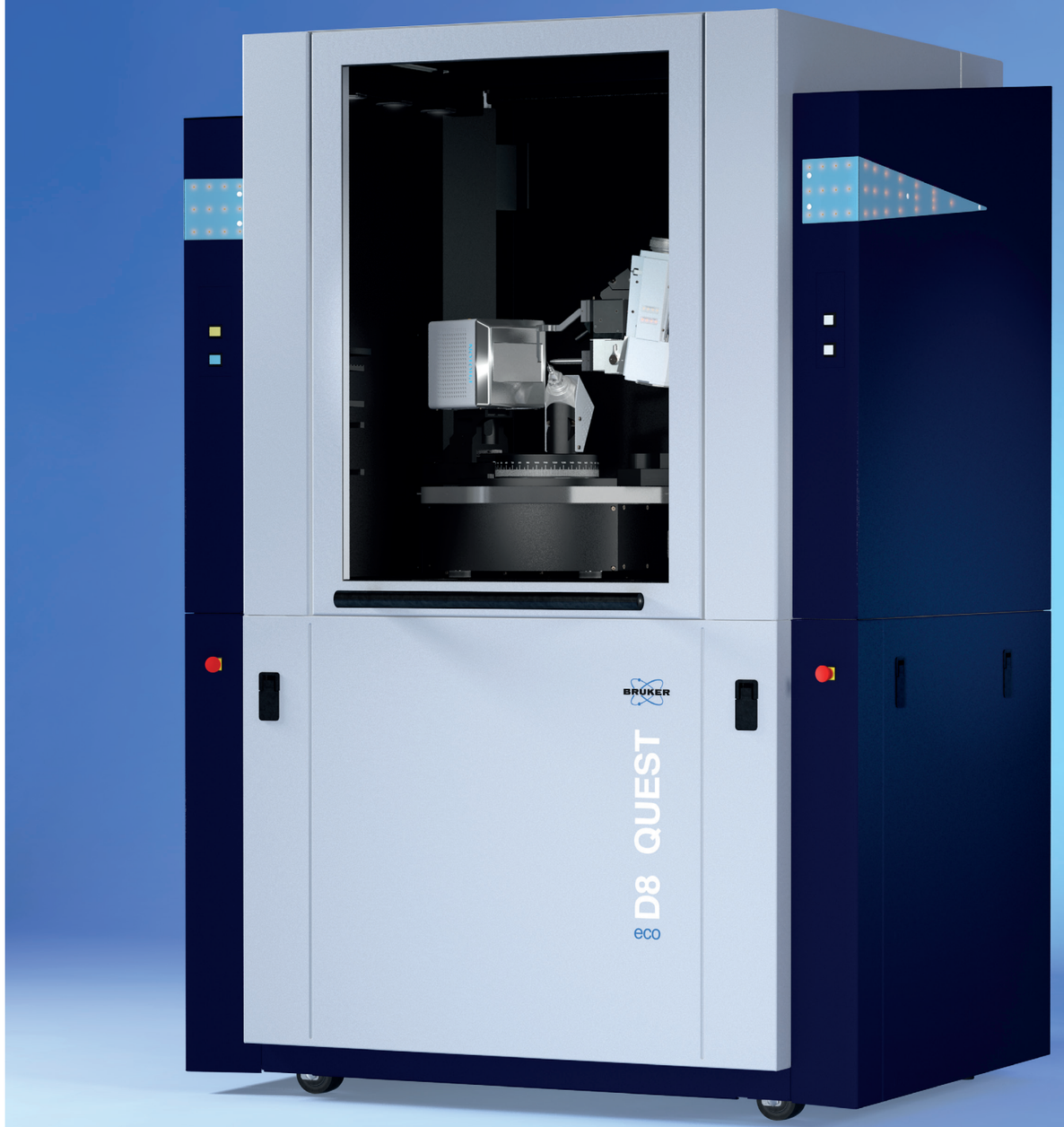
Reliable, low-cost operation

The fixed-chi goniometer is built to last, as has been proven in hundreds of labs, and is equipped with the ultra-stable PHOTON III detector. The X-ray source features highly extended tube lifetimes to bring operating costs to an absolute minimum.

Ready to go

Everything you need for crystal structure analysis is included – diffractometer, control PC, monitor, and the full APEX5 suite of software with unlimited site licenses.

The D8 QUEST ECO is the answer for the laboratory looking for an economical system as the first instrument, or for the established laboratory seeking to expand capacity.



D8 QUEST ECO

Versatile, fully-featured research instrument

Easy crystal mounting

The convenient floor-standing design, with open, fixed-chi goniometer, high-resolution video microscope, and a broad, stable X-ray beam make reliable crystal centering simple.

Short measurement times

Preliminary structures are determined in seconds to allow you to quickly confirm the identity of your sample and search crystal structure databases. Complete data for a fully refined structure refinement is collected in minutes to hours.

Full experimental flexibility

The software-controlled 3-axis fixed-chi goniometer with adjustable detector distance means that complete data is easily collected on crystals of all space groups and unit cell dimensions.

High-quality data

The state-of-the-art PHOTON III 7 detector features photon-counting and a large 7 000 mm² active area to efficiently measure complete data with very high precision, providing the highest-quality experimental data for the most accurate structures.

Publication-quality results

High-quality data makes it easy to determine publication-quality crystal structures. Automated report generation provides all the experimental details and quality criteria to help you write your structure paper.

APEX5 – usability and performance without compromise

The new APEX5 suite offers the most advanced software package for structure determination, convenient sample centering and leading to stunning results with publication-ready reports. APEX5 offers user-selectable levels of automation which allow novice users to quickly learn, while experienced crystallographers can take complete control.

Non-ambient crystallography

Low-temperature devices can be added in the radiation safety enclosure to enable cryo-crystallography. The data collection plug-in of APEX5 even allows for multi-temperature strategies to investigate phase transitions, for example.

Rapid phase ID from powder samples

The broad high-flux, beam and PHOTON III detector mean the D8 QUEST ECO can quickly measure microgram quantities of powder sample without any hardware changes.

Technical highlights

- Full 3-axis goniometer with adjustable 2-theta and crystal-detector distance for full experimental flexibility and complete data sets with Mo- and Cu-radiation
- PHOTON III photon-counting detector with 7 000 mm² active area, highest Detective Quantum Efficiency (DQE)
- Long lifetime fine-focus sealed-tube X-ray source for Mo or Cu radiation
- Unlimited site licenses for the full APEX5 software suite

D8 QUEST ECO in education
Teaching chemistry with crystallography

Crystallography is an important component of the university chemistry curriculum. This powerful technique demonstrates to students that the structure of molecules is 3-dimensional, much different from the 2-dimensional drawings seen in textbooks and classrooms. It clearly conveys ideas like atomic radius, bond length, and chemical structure, from simple covalent bonds to hydrogen bonding motifs and Jahn-Teller distortions.

There is no better way to learn, than by actually doing the experiments yourself. A hands-on approach to learning is the most effective method to develop a deep understanding of crystallography and structural chemistry.

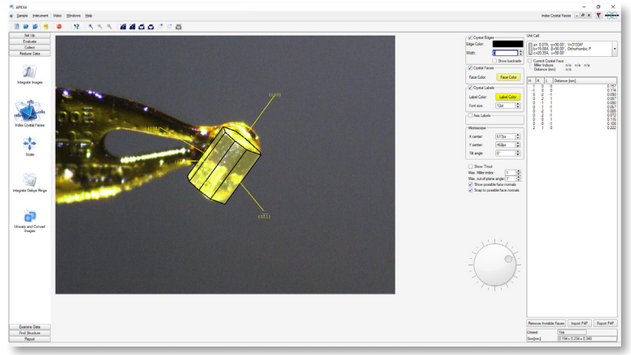
The Bruker D8 QUEST ECO is the ideal solution to meet the specific requirements of the teaching laboratory. Its small footprint and full flexibility allow for a high-quality learning experience.

Benefits of the D8 QUEST ECO for the teaching lab

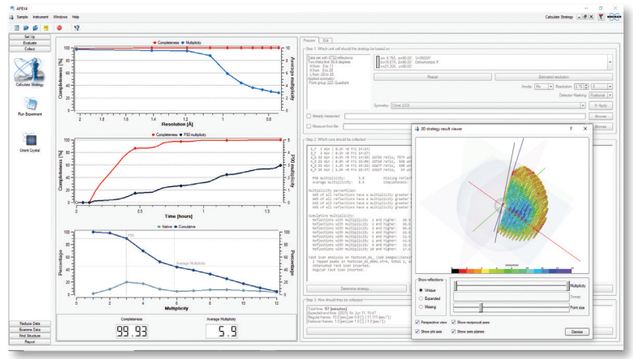
- The system safety interlocks make it impossible for students to be exposed to X-rays.
- The compact design and simple installation mean that the system can be easily accommodated in teaching labs.
- The open goniometer design makes it easy for students to practice mounting and centering crystals.
- Short measurement times provide students with real hands-on training in practical crystallography during a single half-day lab class.

APEX5 - features for teaching

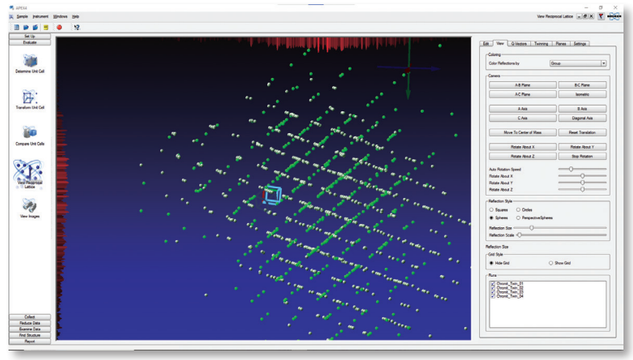
Teachers and students alike appreciate APEX5. Its logical workflow makes it easy for students to understand the key steps of crystal structure determination. The graphical feedback gives students a genuine understanding of why data is collected the way it is, and how the different experimental parameters influence the results.



Crystal face indexing relates symmetry in reciprocal space to real space – the crystal habit



Understand how the data collection strategy is used to measure all the reflections



Understand the crystal lattice in reciprocal space, and explore twin laws

Technical specifications

D8 QUEST ECO	Exterior dimensions	187 × 130 × 114 cm (h ×w ×d)
	Weight	750 kg
	X-ray safety	2 independent fail-safe safety circuits
	Power supply	Single-phase: 208 to 240 V, 50/60 Hz
X-ray source	Type	Fine-focus sealed-tube X-ray source
	Power	1 kW
	Available wavelengths	Molybdenum, Copper
	Monochromator	Triumph monochromator delivers 3× higher flux for Mo
	Cooling	Internal closed-loop water chiller; no external water supply required
Goniometer	**Fixed-chi goniometer**	Software controlled, 3-axis goniometer
	2-theta angular range	Better than -148° to + 159°
	Omega angular range	- 270° to + 270°
	Phi angular range	n × 360°
	Chi angle	54.7° (magic angle)
	Sphere of confusion	<7 µm
Detector	**PHOTON III 7 CPAD**	Indirect, charge-integrating pixel-array detector
	Operating mode	Mixed-mode, photon-counting
	Active area	70 × 100 mm² (h × w)
	DQE	95% (Mo Kα), 99% (Cu Kα)
	Readout deadtime	0.0 ms (shutterless data collection)
	Frame rate	70 Hz
	Sample detector distance	Adjustable 38 – 200 mm with digital distance recognition
Software	**APEX5 software suite**	Most comprehensive software package for single crystal X-ray diffraction using well-tested first-class algorithms Unparalleled ease of use: from data collection and data integration to structure solution, refinement, and publication CIRRUS for user-friendly sample submission and streamlined user and job management.
	Automated structure determination	STRUCTURE NOW provides fully automated data collection, structure determination, and report generation
	Powder analysis	DIFFRAC.EVA processes and analyses 2D powder diffraction data collected on D8 QUEST ECO
	Operating system	Windows for PC
	License provision	Unlimited site licenses provided with the system; free software updates
Optional accessories	Low-temperature device	Various integrated options available for cryo-crystallography
	Automated Goniometer Head	Motorized goniometer head for software controlled 2-click, centering using APEX5
	Diamond Anvil cell	For high-pressure crystallography

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