Software is a crucial part of the investment in a crystallographic system. It provides the interface between you and your diffraction solution. With the new APEX3 software suite Bruker continues its long history of offering the most advanced software package for structure determination, from convenient sample centering to stunning reports, ready for publication.

What does modern crystallographic software do for you?

- APEX3 handles the vast majority of crystallographic challenges, with the right level of automation for the novice, while providing detailed control for the seasoned crystallographer.

- APEX3 is intuitive, easy to learn, professionally supported, and uses world-class algorithms and scientific engines.

- APEX3 is designed following modern Graphical User Interface (GUI) guidelines. Most importantly, the information load reflects the problem, consistency is ensured and the output is clearly presented and self-explanatory.

Is it a surprise? The most popular software is the easiest to use

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

The APEX3 GUI guides you through the complete experiment with minimal input and maximum graphical feedback, focusing on the structure determination at hand. The GUI follows the natural flow of the experiment, transferring information from step to step, and auto-filling dialog boxes. At all times, the GUI keeps you informed about the progress and quality of the structure determination process. The underlying engines for data acquisition, unit-cell determination, data integration, and scaling utilize the world’s best algorithms to generate superior data. You will benefit from built-in expert knowledge about instrument geometry and data collection strategies.
APEX3 sets new standards for usability and performance

Bruker’s new APEX3 software suite is the only package that includes all the engines, routines and programs you need from controlling the instrument to publishing the refined structure. Be it a routine structure or a challenging crystallographic problem, APEX3 seamlessly integrates the world’s most powerful software modules to give you a complete and comprehensive state-of-the-art package.

The reliable and consistent package from a single provider
Where other user interfaces only serve as an artificial and restrictive shell, haphazardly thrown together over a collection of public domain programs, APEX3 provides seamlessly integrated functionality – fully supported by professionals. Bruker is the only provider of crystallographic systems that does not rely on public domain software but heavily invests in the resources to develop this essential component providing the world’s best solutions in Single-Crystal X-ray Diffraction.

From crystallographers for crystallographers
APEX3 has been conceived and created by crystallographers for crystallographers. APEX3 is the most comprehensive crystallographic software suite which has been continually developed, tested and improved since the early 2000s. Bruker maintains the professional environment that is essential to support software projects of this magnitude and ensures that software development follows stringent industry standards. To quickly react on new trends Bruker’s software group employs agile methods with short iteration cycles to guarantee shortest time to market. Before it is deployed, each release is thoroughly tested by a large team of applications scientists and selected beta sites around the world. Customer access to software is easy and fast through downloads from Bruker’s support site at brukersupport.com.

With the acquisition of a Bruker diffractometer you do not only purchase a piece of hardware, you will acquire a complete diffraction solution that is intuitive and easy to use and delivers results that make your research excel. This is where APEX3 comes into play – the collective knowledge of many crystallographers condensed into an amazing suite of crystallographic software.

Getting started – Welcome to APEX3
APEX3 follows the natural flow of the experiment turning structure determination into a very intuitive process. It all starts with mounting and centering the sample in the X-ray beam. The next steps can be fully automated or be done with you in full control using varying degrees of automation. Does the sample diffract? How strong is the diffraction signal? Is it a good quality sample? Is it a single crystal or a twin? APEX3 helps you answer these questions with a wealth of tools or automated routines. Cell determination comes with the three most successful indexing routines the crystallographic community has developed and two of those are exclusive to Bruker. What if your crystal is a twin, incommensurately modulated or an intergrown sample? No worries, these more challenging cases are all covered by the suite. Convenience, transparency and efficiency – these are the concepts our programmers

Did you know that Intrinsic Phasing …

- solves 52% of the structures entirely correct
- solves 19% of the structures with just one atom incorrectly assigned
- solves 13% of the structures with only two atoms incorrectly assigned
- anecdotally never missed an atom
- assigns the space group correctly in more than 98% of the cases

Marilyn Olmstead, UC Davis. Chiral Cage of C68 with Sc3N inclusion. Fullerene with three sets of pentalenes that violating the ”isolated pentagon rule”
Scaling and absorption correction

Excellent data requires first-rate scaling and the increased use of copper radiation for small molecule crystallography has raised the importance of proper absorption correction. Numerical methods are typically seen as a prerequisite for producing excellent data and this approach requires that a crystal’s shape is accurately described by indexing the crystal’s faces. APEX3 has all easy-to-use-tools for face indexing, automated whenever possible and applied where applicable. However, often crystal faces are not defined well enough to be accurately indexed and measured. That’s when multiscan methods shine, producing high quality hkl-files for further processing. Multiscan methods are implemented for single crystals, modulated and twinned data.

From spots to intensities

Reflections have a three-dimensional intensity distribution. Our software is dedicated to preserving this information, carefully extracting the 3-D spot profiles from finely sliced diffraction images. This provides the best possible way to process weak reflection intensities. Particularly for challenging samples – where every reflection counts – this approach makes a big difference, and our data quality always prevails. APEX3 is the only package that applies profile information for twinned, split, or modulated crystal data. APEX3 supports data formats from select synchrotron beamlines.

APEX3 is designed with a framework concept that connects its plugins through a PostgreSQL database. This approach keeps plugins independent but ensures reliable communication and exchange of data.

Did you know that the database …

- lets plugins communicate with each other, ensuring transparent data import and export
- stores all experimental data relevant to the project, and ensures data consistency and integrity
- is at the heart of report generation and ensures that reports are always up-to-date
- keeps a history, and provides the reliable archiving of your projects
- controls user management, and user access to projects
- facilitates connecting your diffraction solution to an existing LIMS system

Published Structures in Acta E 2005 – 2014

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1) Supplier search results Acta Crystallographica Section E
Search terms: “Bruker” = “Bruker” or “Siemens” or “Nonius” not ("Bruker Nonius" or "Bruker-Nonius")
“Rigaku” = “Rigaku”
“Agilent” = “Kuma” or “Oxford” or “Varian” or “Agilent”
Everybody on Stage! Fully Integrated Design

Image Analysis
The intuitive APEX3 diffraction image interface provides all the means for image analysis, including: zoom and panning, 3-D views, line graphs, rocking curves, resolution rings, and many more. These tools make judging data quality or investigating problem cases easy and efficient.

Unit Cell Determination
A unique combination of Fast Fourier, Difference Vector and Least Squares techniques helps indexing the most difficult data reliably. 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. This is especially important for those low symmetry cases and longer wavelengths that require a lot of data to high diffraction angles to reach atomic resolution. Confidently rely on automated strategy determination that lets you adjust parameters and lets you be in the driver seat.

Data Integration
True 3-D integration with algorithms optimized for narrow and wide scans with full support of shutterless data collection result in unsurpassed data quality, fastest integration software for standard structures and more challenging data like twins and incommensurates. On-the-fly integration provides intensive feedback including integration progress and quality, 3-D reflection profiles, multiple component spot overlays, and many more...
With All Engines Required

Scaling
Scaling is the important final step of data reduction and will provide you with the data used for structure determination. The scale plugin does so much more than scaling. It also corrects for absorption and adjusts the error model on request. The plugin handles single crystals, twins and incommensurates, all transparent to the user. Graphical feedback and intelligent parameter suggestion make this very complex task accessible to the novice.

Structure Solution
This plugin wraps around George Sheldrick’s programs for structure solution and offers classical Direct Methods and Patterson techniques, advanced dual space methods and the truly ingenious Intrinsic Phasing approach. The plugin provides easy parameter control for these methods and displays the structure found as well as the pertinent reliability and structure quality parameters. Structure solution for chemical crystallography has never been easier.

Automated Structure Determination
New to crystallography or pressed for time? Just specify the formula, and let XPRESSO do the rest. The module will automatically determine the quality of your sample and plan the best data collection strategy, process all data, and solve and refine the structure. The module provides molecular graphics and a complete HTML report with all tables and information necessary for publication.

Face Indexing
Built to dimension! 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 Evaluation
It doesn’t always have to be a single crystal. You can also use your single crystal diffraction system for collecting and processing good-quality powder diffraction data. The plugin handles diffraction from polymers, fibers and partially oriented powders and provides export to the full suite of Bruker XRD software.

Reciprocal Lattice Viewer
The plugin helps to display and interactively modify reflection arrays. Removing artifacts from strong amorphous scatterers or visually separating twin components and determining q-vectors of incommensurates are easily achieved. The reciprocal Lattice viewer is a powerful tool for tackling the most challenging crystallographic problems.

Diffraction Space Viewer
Diffraction from a different angle! Display the complete reciprocal space as a volume reconstructed from diffraction images. The module allows investigation of textured samples, fibers and non-Bragg diffraction. The GUI provides free rotation, zoom, and display of slices.

Structure Refinement
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 both for the novice and the expert. Electron density maps let you look beyond the spherical model and let you capture minute details of your structure.
Overhead time minimized to zero

Did you know that PLATON ...
- checks refined structures for omissions & obvious errors, including misplaced hydrogen atoms, in data sets prior to the submission to a journal
- points to technical shortcoming, such as impacts arising from pseudo-symmetry, disorder and many others
- is a great tool for determining unusual - but potentially interesting - structural features like unusually short intermolecular contacts

Did you know that the new AUTOSTRUCTURE ...
- determines 87% of all structures entirely correct
- integrates the electron density around an atom after the anisotropic refinement to locate hydrogen atoms
- is tested against 1584 structures taken from the Crystallography Open Database (COD)

Our modern CMOS detectors allow for shutterless data collection. This makes data collection faster than ever before, while improving data quality at the same time. APEX3 fully supports shutterless data collection. This includes setup, data processing and scaling of fast scans. Like beam attenuators that were used in the past the fast scans increase the dynamic range of the system and allow measurement of strong reflections next to very weak intensity signals.

The table below compares important reliability criteria from data that we collected using the conventional “shuttered” data collection mode, the shutterless data acquisition mode and shutterless data using additional sets of frames with the idea to improve data quality by increasing multiplicity.

Within small limits, the quality of the structure of sucrose that was refined against shutterless data matches that for the structure refined against data acquired in “shuttered” mode. However, in this case the data collection was accomplished 3.5 times faster. While collecting twice as many reflections, still in shorter wall-clock time compared to the original, “shuttered” mode, the structure could be improved impressively in shutterless mode.

Reliability criteria for sucrose data sets obtained using “shuttered” and shutterless data collection modes (1 second exposure time)

<table>
<thead>
<tr>
<th>Mode</th>
<th>Shutter</th>
<th>Shutterless</th>
<th>Shutterless (higher multiplicity)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment time</td>
<td>35 min</td>
<td>10 min</td>
<td>20 min</td>
</tr>
<tr>
<td>Relative time</td>
<td>3.5</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Refl. Total/Unique</td>
<td>8315/3472</td>
<td>8431/3470</td>
<td>16873/3507</td>
</tr>
<tr>
<td>Flint [%]</td>
<td>1.35</td>
<td>1.30</td>
<td>1.48</td>
</tr>
<tr>
<td>Flsig [%]</td>
<td>1.58</td>
<td>1.56</td>
<td>1.08</td>
</tr>
<tr>
<td>Flpim [%]</td>
<td>1.61</td>
<td>0.90</td>
<td>0.63</td>
</tr>
<tr>
<td>R1 [%]</td>
<td>2.14</td>
<td>2.13</td>
<td>2.06</td>
</tr>
<tr>
<td>wR2 [%]</td>
<td>5.51</td>
<td>5.62</td>
<td>5.55</td>
</tr>
</tbody>
</table>

C. Wandtke*, H. Ott*, B. Dittrich*, *University of Goettingen, #Bruker AXS Karlsruhe: Electron density study on Lincomycin, electrostatic potential shown (to be published)
APEX3 – Enjoy the feeling

Relax and stay tuned
Even though the introduction of the most sensitive CMOS APS sensors and ever stronger X-ray sources has significantly decreased the need for lengthy diffraction experiments, all our diffraction solutions are designed for long-term unattended operation. Consequently, with APEX3 there is no need for waiting next to the instrument once the sample is properly centered and all doors are closed. Thanks to Bruker’s unique client-server setup you can access your instrument from the computer next to the instrument, from your office next door, from the 10th floor of the neighboring building, from home, or even from the whitest beach or the highest mountain. Our proprietary protocol based on TCP/IP allows easy, safe access from just about anywhere! And, why not give the XPRESSO automation a try? Just press a button, take a coffee, and let APEX3 do all the hard work. In addition the new APEX3 software suite reliably informs you via email once the instrument is ready for the next challenging sample. Do you prefer working on the most important structure offline away from distractions? Simply take your Windows or Linux APEX3 laptop to your favorite place, process the data, refine the structure, create all required reports and graphics within the very same suite.

The Bruker Users group — a really special thing
In addition to the APEX3 software support provided via our service support, a very active Bruker users’ group is established. With the introduction of 2D electronic detectors for the home-lab, our customers started this group, which has grown to about 600 members, including a large number of world-class crystallographers. The group is actively exchanging hints and tips addressing crystallographic challenges such as twinning and modulation. As these are global groups you can expect replies virtually on a 24/7 basis, with someone always reading the mails somewhere. In practice this means that urgent questions can be answered almost instantly and your research can progress without delay. Become part of the global Bruker family in crystallography and join the community of Bruker users.

D. Ananias, F. A. Almeida Paz, D. S. Yufit, L. D. Carlos, J. Rocha J.
Am. Chem. Soc., 2015, 137 (8), pp 3051–3058
DOI: 10.1021/ja512745y
What users say ...

“The APEX software package nicely takes care about all parameters required for the different wavelengths and the entire data processing is easy to perform, nicely transparent and delivers good results in almost no time.”

Sine Larsen, Professor in structural chemistry, former IUCr president and Director of Research at ESRF, University Copenhagen

“In addition to the hardware, we are very happy with the performance of the APEX3 software suite included with each of the systems. Expert crystallographers appreciate the ability to fine-tune parameters of the underlying engines used at the different stages of the structure investigation process. On the other hand, occasional users find the software easy to handle as it immediately gives access to tools for automated data collection and structure solution.”

Dr. Stanislav Pachev Institute of Condensed Matter Chemistry of Bordeaux – CNRS Bordeaux, France

“In the old days it was a real challenge to investigate twinned, intergrown or modulated samples. With the modern APEX3 software such problems are tackled with ease.”

Prof. Bohari M Yamin, School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, Bangi, Malaysia

“The D8 QUEST and the superb APEX3 software suite enabled us to solve and refine the crystal structure of a tiny, very weakly diffracting photoluminescent lanthanide silicate with high quality”

Prof. Dr. Filipe A. Almeida Paz, University of Aveiro, CICECO, Department of Chemistry, Portugal

APEX3 – The New Highlights

Most comprehensive software package for single crystal X-ray diffraction (SC-XRD) using well tested first-class algorithms.

Unparalleled easy-to-use at all steps: from data collections and data integration to structure solution, refinement and structure publication.

Intrinsic Phasing (ShelXT) solves the vast majority of structures in seconds with no space group input required.

Improved twin handling of up to eight domains with excellent graphical feedback and easy determination of the twin law.

New model refinement plugin for interactive graphical visualization of the three-dimensional structure including electron density and difference density maps.

Autostructure delivers the entirely correct structure in 87% of all cases.

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