MS3-P4 Reaching a new highpoint with crystallography software - APEX3

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In 2004, the APEX2 single crystal suite was first launched and deemed a huge leap forward in terms of functionality and design, compared to previously available software. This suite allowed for complete crystal structure determination, from data collection on the instrument to finalization of a publishable structure, to be completed within one program. Since its launch, the performance of the APEX2 suite has been continuously enhanced by the addition of various features. Today it is one of the most popular software suites used in chemical crystallography. Now, the most extensive revision is available: APEX3. This major new release takes full advantage of important developments in computer hardware and operating systems. Improvements to the new package include a state-of-the-art graphical user interface built with the modern QT4 development framework, updates to faster versions of Python and the PostgreSQL database as well as multi-CPU support for faster data processing, structure solution and reporting.
The updated AUTOSTRUCTURE plug-in makes full use of the revolutionary Intrinsic Phasing structure solution engine, increasing the out-of-the-box success rate of structure determinations far beyond 90%. The new Structure Determination plug-in incorporates various structure solution modules, including SHELXT, while ShelXle is fully incorporated as the new default option for fast and convenient structure refinement. Moreover, the efficient twin handling routines known from the APEX2 suite are now fully integrated into the GUI for a new level of seamless twin support. APEX3 extends the ease of use of APEX2, and is readily learned by new users and students alike, keeping the focus on learning the science of crystallography.

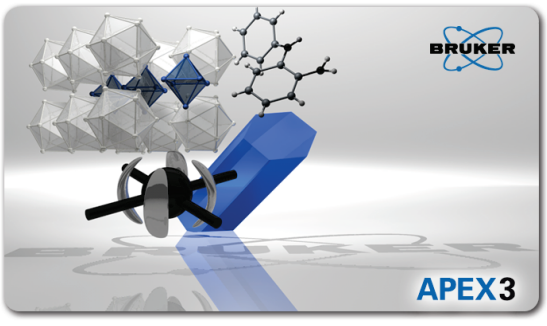

Figure 1. APEX3 Splash screen

Keywords: comprehensive crystallography software, easy-to-use, most popular suite, automated structure solution, SHELXTL

MS4. Advances in phasing, refinement, and autobuilding

Chairs: Navraj Pannu, Eleonor Dodson

MS4-P1 BRICKWORX builds recurrent rna and dna structural motifs into medium and low-resolution electron density maps

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BrickworX is a computer program that builds crystal structure models of nucleic acid molecules using recurrent RNA motifs extracted from RNA Bricks database (http://iimcb.genesilico.pl/rnabricks) or B-DNA double helices. In a first step, phosphate groups are detected in a user-provided electron-density map. Subsequently, comparing the three-dimensional patterns of the P atoms with a database of nucleic acid fragments, matching positions of the motifs in the unit cell are found. Finally, the matched motifs are merged and refined in real space to find the most likely conformations, including a fit of the sequence to the electron-density map.

The Brickworx program is available for download and as a web server at http://iimcb.genesilico.pl/brickworx.