MS3-P1 **Crystal shape recognition software** Václav Eigner,[ab] Michal Dušek,[b] Jan Čejka,[a] [a] *Department of Solid State Chemistry, Institute of Chemical Technology, Technická 5, 166 28 Prague, Czech Republic,* [b] *Institute of Physics AS CR, v.v.i., Na Slovance 2, 182 21 Prague 8, Czech Republic*
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The X-ray structure determination has seen fast development over last twenty years from a special method towards a semi-automatic tool available to any sufficiently trained scientist. Despite the advancements in both the instruments and methods, some materials still resist the routine approach. Multi-domain crystals with strong x-ray absorption are frequent cases in this category, because absorption degrades precision of diffraction data and creates significant differences between symmetrically equivalent reflections. In case of multidomain samples the situation is furthermore complicated by the presence of overlapping reflections, and also by shading one domain by the others. Typical examples of highly absorbing materials are minerals containing heavy elements, but high absorption is also encountered with moderately heavy elements measured with copper radiation.

Although the commonly accessible diffractometer programs usually contain tools for absorption correction, details of their functionality are unknown. Moreover, such absorption correction cannot be undone and repeated in later stages of structure solution when the data are processed by different software. For this reason we have started a project [1] of moving absorption correction tools into Jana2006 software [2]. Here we present the first successfully finished part, a tool for automatic shape indexing.

The presented Crystal shape recognition software uses as an input photographs of the crystal shape acquired for various orientations of the sample with the program Crysalis [3], which is delivered for laboratory diffractometers produced by Agilent (former Oxford Diffraction). In Crysalis, the user defines crystal faces by dragging lines with the computer mouse and then the program assigns them *hkl* indices. In our software the same operation is done automatically, based on the contrast between the image of the crystal and the background. For small samples where the pixel size limits the precision of the mouse movement, this method is more precise. In the next step, the user can make manual corrections of the preliminary shape with a step unlimited by the resolution of the frame. Currently, we are implementing this program to the Jana2006 software [2].

[1] Czech Science Foundation P204/11/0809.
[2] Petříček, V., Dušek, M., Palatinus, L., (2006). Jana2006. The crystallographic computing system. Institute of Physics, Praha, Czech Republic.
[3] CrysAlisPro, version 1.171.35.21, Agilent Technologies (2012).

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MS3-P2 **New Tools for Biological Crystallography in the Home Lab: results.** Severine Freisz,[a] Vernon Smith,[a] [a]*Bruker AXS GmbH, Östliche Rheinbrückenstr. 49, Karlsruhe (Germany).*
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Advances in crystallographic hardware and software have enabled structural biologists to investigate more challenging projects. Recent developments have greatly increased the capabilities of in-house diffraction systems providing increased productivity for synchrotron trips and home-lab studies.

The latest improvements in source and detector technology have significantly improved the capability of home-lab systems for both screening and data collection.

We have now introduced the new D8 VENTURE solution for Structural biology with the new PHOTON 100 detector, the first CMOS active pixel sensor for X-ray crystallography. The new TXS and IμS, now deliver beam intensities comparable to those of typical bending-magnet beamlines.

Here we present the results obtained on usual test crystals like lysozyme, thaumatine and insulin as well as on "real life" crystals.

Biology; Crystallography; CMOS; Home-lab system