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Automatic Absorption Correction for an Arbitrary Shaped Crystal from Digital Images. E.A. Zhurova¹, V.V. Zhurov², K. Tanaka³, V.G. Tsirelson⁴, ¹Univ. of Toledo, Toledo, OH 43606, USA, ²Karpov Inst. of Physical Chemistry, Moscow 103064, Russia, ³Nagoya Inst. of Technology, Nagoya, Japan, ⁴Mendeleev Univ. of Chemical Technology, Moscow, Russia.

A method and the CCDABS software have been developed to automatically reconstruct the 3D-shape of an arbitrary crystal from a set of digital images, and to calculate the absorption correction for X-ray diffraction data. The procedure consists of edge-preserving image smoothing using a variation of the anisotropic diffusion method, edge detection, determination of the crystal boundaries, capillary and glue parts subtraction, and definition of the 3D crystal surface as two sets: (i) restricting



planes and (ii) points in polar coordinates. A special procedure was developed for fast integration of absorption coefficients over the crystal volume. The CCDABS software can operate in both automatic and manual modes. The program was tested using simulations of various shapes. Finally a KMnF₃ sample (0.108x0.145x0.195 mm, 1889 reflections collected over the full reflection sphere with statistical accuracy of 0.5%) was used. For the most influenced reflections, the internal R-factor was 1.0% after correction compared to 2.7% without it. For the complete reflection set, values of 1.1% and 2.2%, respectively, were obtained.