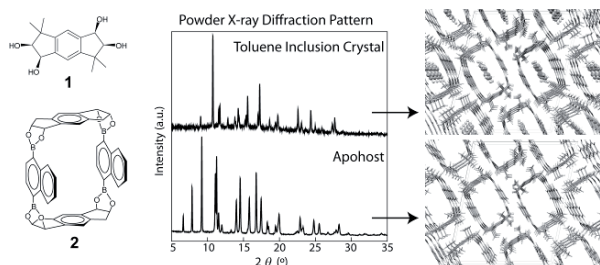


study, the apohost of **2** was determined from the laboratory powder X-ray diffraction data and the structural change by guest sorption and release processes were investigated.

The powder X-ray diffraction data of the toluene inclusion crystal of **2** and the apohost crystal of **2**, which was obtained by heating of the toluene inclusion crystal, are significantly different as shown in the figure. However, interestingly, the apohost structure, determined from the laboratory powder X-ray diffraction data, was found to retain its crystal packing even after the guest release. The apohost has one dimensional stacking of **2** along the *b*-axis forming the one dimensional guest free tunnel. This tunnel is expected to absorb the guest molecules easily and, in fact, the apohost crystal readily absorbs the toluene molecules, when the toluene vapor was applied to the solid apohost, and it transforms into the toluene inclusion crystal within 20 min.



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Keywords: *ab-initio* powder structure determination, solid-state transformation, macrocyclic compound

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Highly automated synchrotron beamline dedicated to SAXS on proteins in solution

Louiza Zerrad,^a Petra Pernot,^a Vicente Rey-Bakaikoa,^a Adam Round,^b Florent Cipriani,^b Alexandre Gobbo,^b Julien Huet,^b. ^a*European Synchrotron Radiation Facility, ESRF, Grenoble (France)*. *European Molecular Biology Laboratory, EMBL, Grenoble (France)*. E-mail: louizazerrad@esrf.fr

Introduction of the new generation sample changer on the recently rebuilt BioSAXS ID14-3 beamline at the ESRF together with the implementation of 1M Pilatus detector have sensibly boosted its high-throughput capacities. The sample changer developed in collaboration between the ESRF and the EMBL (Grenoble and Hamburg outstations) automates the entire cycle of sample loading-unloading-cell cleaning and can hold up to several hundred of samples in micro-plates, eppendorf strips (PCR) or tubes. Thermal control, smart pipetting and sample positioning together with other features allow to run completely automated data collection without any user intervention through the dedicated beamline software, BsxCuBE. The user just needs to enter sample information (name, concentration, location in sample changer, etc.) and collection parameters (exposure time, temperature, flow during exposure, etc.). Afterwards the script performs data collection in the most economical and safe manner, processes 1D curves and filters them according to the radiation damage. It is followed by automated processing pipeline (developed by EMBL Hamburg) which analyses 1D curves and gives structural properties of the proteins (molecular sizes and *ab-initio* models). Reliable and simple-to-use sample environment together with robust software allow to perform easily and efficiently the SAXS experiments even by non-experienced users.

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Keywords: SAXS-1, Automation-2, Biomacromolecules-3

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An automated sample environment for biological solution scattering experiments at 3rd generation synchrotrons

Florent Cipriani,^a Franck Felisaz,^a Lukas Fodinger,^a Alexandre Gobbo,^a Julien Huet,^a Raphael Moya,^a Cyril Villard,^a Adam Round^{a,c}, Manfred Roessle,^b Dmitri Svergun^b; Petra Pernot^c. ^a*European Molecular Biology Laboratory, Grenoble Outstation, (France)*, ^b*European Molecular Biology Laboratory, Hamburg Outstation, (Germany)* ^c*European Synchrotron Radiation Facility, (France)*. E-mail: cipriani@embl.fr

Small-angle X-ray scattering for macromolecules in solution is widely used in structural biology to complement high-resolution structure determination obtained by x-ray crystallography or NMR. In the context of third-generation synchrotron sources, this increasing interest leads to developments of automated sample environments. Based on the background acquired at the EMBL Hamburg X33 beamline, a collaboration has been established between the EMBL and the ESRF to develop a system able to expose automatically to x-rays micro-volumes of solution with minimum time overhead. The key concept to reach this objective was to minimize length of the fluidic path, using an architecture where the exposure cell is connected to a fixed pipetting needle with very short tubing, and where the sample wells are moved to the needle. With this system, several hundred samples stored at controlled temperature in strip wells or in SBS Microplates can be automatically loaded for exposure to x-rays in a vacuum mounted and temperature controlled glass capillary. Volumes of solution down to 5 μ l can be reliably exposed to an x-rays beam in flow mode. After exposure, the fluid path is cleaned and dried automatically in less than 20 seconds. Several thousand experiments have been carried out at the ESRF ID14-3 beamline, the EMBL Doris X33 beamline and the EMBL@PETRA-III BioSAXS beamline. The liquid handling features of the machine associated with an in-line spectrometer allows for sample concentration measurement, dilutions or additions. Efficient use of the small and intense x-ray beams available at 3rd generation synchrotron is now possible using this new automated sample environment, in particular when associated with the last generation of fast counting silicon pixel detectors.

Keywords: SAXS, high throughput, sample changer

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Structural changes in DL-serine under hydrostatic pressure up to 4.3 GPa

Boris A. Zakharov,^{a,b} Boris A. Kolesov,^c Elena V. Boldyreva,^{a,b} ^a*REC-008, Novosibirsk State University, Novosibirsk*. ^b*Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk*. ^c*Institute of Inorganic Chemistry SB RAS, Novosibirsk (Russia)*. E-mail: b.zakharov@yahoo.com

The studies of molecular crystals at non-ambient conditions (low temperatures and high pressures) help to understand intermolecular interactions and their role in the formation of crystal structures and