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.


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

MS11.P01  
Highly automated synchrotron beamline dedicated to SAXS on proteins in solution

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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 has 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, 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.


Keywords: SAXS, high throughput, sample changer

MS12.P01  
Structural changes in DL-serine under hydrostatic pressure up to 4.3 GPa

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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