$ZnCl_2$ or other metal cation versions[3].

Final products are polycrystalline and usually containing several novel crystalline phases of uncertain chemical composition, so we performed synchrotron high temperature *in-situ* powder diffraction measurements on prepared compounds (T-ramping)[4]. Structure solution was carried out by combining information obtained from electron density maps provided by Direct Methods and several direct space approaches such as Simulated annealing and Parallel tempering[5].

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Keywords: metal-hydride organic frameworks, mechanochemistry, in-situ powder diffraction

MS37-P2 New high-symmetry layered cocrystal of tetranuclear zinc benzoate

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Zinc-oxocarboxylates are well-known compounds as possible catalysts or luminescent materials [1]. Tetranuclear oxo clusters are in the center of interest because of their role as secondary building blocks in metal-organic frameworks (MOFs) [2]. MOFs with high porosity are widely studied as storage materials for small molecules. Despite of this property there is a lack of studies of intermolecular interactions in simplified systems of building blocks of the frameworks. Detailed study of the supramolecular interactions in high-symmetry tetranuclear zinc benzoate cocrystal helps to understand the nature of basic interactions between the host frameworks and guest molecules in MOFs. Fullerene molecules are good candidates to study supramolecular interactions because they have the ability to form various cocrystals with high-symmetry organic and metal-containing molecules [3].

Here we show the preparation, crystal structure and thermal stability of a new high-symmetry fullerene-zinc benzoate cocrystal. C_{60}-basic zinc benzoate cocrystal was prepared from toluene solutions of the constituents by slow evaporation of the solvents. The trigonal structure of the single crystals consists of alternating fullerene and basic zinc benzoate layers. Fullerenes are ordered in a hexagonal closed packed sheet at room temperature in which all fullerenes are surrounded with six adjacent C_{60} molecules with center-to-center distances similar to distances in neat C_{60} crystals. The monomolecular fullerene layers are fully separated from each other by layers of ordered benzoate molecules. This complex supramolecular assembly is stabilized by incorporated solvent molecules. The thermal stability study based on thermogravimetry mass spectrometry shows that two sets of solvent molecules are built into the cocrystals. In the oxocarboxylate layers strongly bonded toluene molecules are built in between benzoate groups of adjacent molecules. Further disordered toluene molecules with weaker interaction can also be found in the structure.

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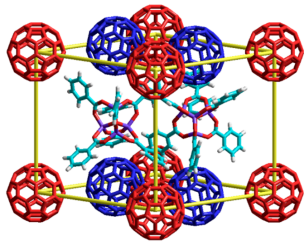

Figure 1. Layered crystal structure of C_{60}-basic zinc benzoate corystal

Keywords: MOF, fullerene, cocrystal

MS37-P3 Alternatives to "co-crystal – salt" transitions in glycine co-crystals at low temperature and high pressure: two new examples as a follow-up to a glycine – glutaric acid study

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The effects of temperature and pressure on the co-crystals of glycine with DL-tartaric and phthalic acids (**GT** and **GP**, respectively) have been studied by X-ray diffraction and Raman spectroscopy in a comparison with those in **GG**. Like for **GG**, for both **GT** and **GP** neither cooling nor increasing pressure resulted in a co-crystal to salt transition. On cooling, no phase transitions were observed in **GT** or **GP**, contrasting the situation with **GG**. On hydrostatic compression both **GT** and **GP** underwent reversible phase transformations, accompanied by fracture. In the high-pressure phases the main structural framework was preserved, the number of crystallographicaly independent molecules in the unit cell increased; the type of intermolecular H-bonds linking DL-tartaric molecules into dimers in **GT** changed in every second dimer from hydroxy-group to hydroxy-group in the low-pressure phase for the hydroxy-group – carboxy-group in the high-pressure phase.

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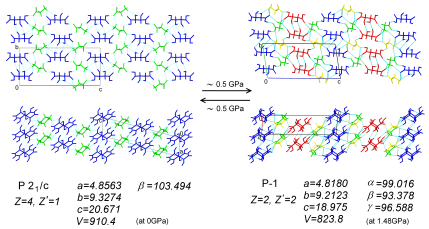

Figure 1. Structural changes in GT due to the phase transition at high pressure.

Keywords: glycine, co-crystal, hydrogen bond, high-pressure