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Single crystal transformations

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Changes in solid state structure due to solvent loss or uptake are common. However, mechanical stress caused by such changes usually results in extensive fracturing of the crystals to yield a polycrystalline powder. In only a handful of cases it has been observed that single-crystal to single-crystal transformations can occur despite relatively large changes to the packing mode of the host framework. Such processes are presumed to involve cooperativity of molecules throughout the crystal during the transformation. These phenomena can be utilized in order to gain a better understanding of dynamic processes in crystals, and can be exploited for applications such as sensors. We have recently embarked on a systematic study of monocrystalline phase transformations as part of our ongoing interest in developing porous materials, and new results in this area will be presented.

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Fluorinated phenoxysubstituted triazines as organic zeolites

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In the last years, many efforts have been made to develop new organic zeolites [1]. Compared to inorganic zeolites, the organic porous structures feature advantages such as diversity on the molecular level (supramolecular synthons) and variability on the supramolecular level (properties of pores). However, these materials generally show a rather low thermal stability. Only a few compounds based on weak intermolecular interactions are known to form channel structures with a persistent porosity. Two recent examples are tris(*o*-phenylenedioxy)-cyclotriphosphazene (TPP) [2] and 2,4,6-tris(*p*-bromophenoxy)-1,3,5-triazine (BrPOT) [3]. In the case of BrPOT a zeolite-like behaviour up to 70°C could be demonstrated. By fluorination of BrPOT we could increase the thermal stability: The fluorinated counterpart 2,4,6-tris(4-bromo-3,5-difluorophenoxy)-1,3,5-triazine (Br-3,5-DFPOT) shows a thermal stability up to about 110 °C investigated by temperature dependent powder X-ray diffraction. This new organic zeolite gives rise to a number of inclusions with varying guest molecules. One example is the sorption of gases such as N₂. Further examples involve the inclusions of functional molecules. Here, it was possible to include the buckyfullerene C₆₀(Me)₅Fe₂c₁₈p [4], whereby polarity formation was found. Furthermore, rather high dark-conductivities were observed for co-inclusions of fullerenes (C₆₀ / C₇₀) and dexamethylferrocene.



Figure: Channel structure of Br-3,5-DFPOT.

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