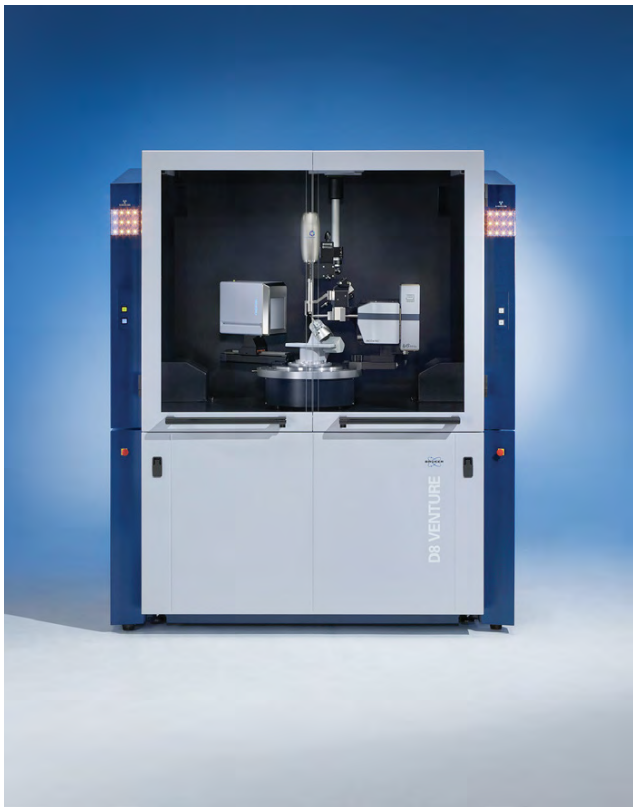

Keywords: in-house solution, synchrotron, automation

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1-Hydroxypyrene under pressure - crystal morphology affected by hydrogen bond

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We have investigated single crystals of 1-hydroxypyrene. This is a relatively uncomplicated crystal structure, where monoclinic unit cell consists of four molecules, kept together by O-H...O hydrogen bonds and π-stacking intermolecular interactions. These interactions, as well as characteristic features of 1-hydroxypyrene molecules, such as conjugated aromatic rings, strongly affect the crystal morphology.

It is already known, that the morphology of a particular crystal can be assessed with the use of the attachment energy model [1]. There are also papers describing influence of solvent environment on crystal morphology [2,3].

In the case of 1-hydroxypyrene, when single crystals are grown from non-polar solvents such as n-pentane or n-hexane, they crystallize in form of long, thin needles. Calculations of the attachment energy confirm this morphology. However, when single crystals of 1-hydroxypyrene are grown from polar solvents such as methanol or acetone, they crystallize in form of plates.

What is more, we have also performed crystallization of 1-hydroxypyrene under pressure, with the use of Diamond-Anvil Cell (DAC). Surprisingly, this experiment has revealed that under pressure, even where polar solvent was used, 1-hydroxypyrene again crystallizes in the form of needles, which are extremely flexible. Crystals are so pliable that during crystal-growth they can easily bend, even about almost 90 degree, rather than grow thicker. This behavior of crystals in DAC reveals dominant influence of hydrogen bonds on morphology of the crystal, and suggests, that the role of the solvent's polarity in crystallization process diminishes with pressure. Molecules of 1-hydroxypyrene form substructures which are kept together by above-mentioned hydrogen bonds. Such substructures resemble columns where aromatic rings of neighbouring molecules form π-stacks, thus enhancing the effects of H-bonding. These columns coincide with the long direction of the needle and allow it for the crystal's flexibility. It can also explain negligible compressibility with pressure in that particular direction in the crystal lattice.

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Keywords: high pressure, hydrogen bond, crystal morphology