Electronic Supplementary Material (ESI) for CrystEngComm

Supramolecular structure of ammonium polyoxoarsenates(III)

Piotr A. Guńka, Maciej Dranka* and Janusz Zachara

Supporting Information

Morphology of crystals

Predicting morphology of crystals is a very demanding task due to numerous factors determining the final habit. Periodic Bond Chain (PBC) theory can be applied to systems with a combination of strong and weak interactions in order to predict the habit of crystals grown in such conditions that internal factors (*i.e.* structure) are the only factors determining the habit[1].

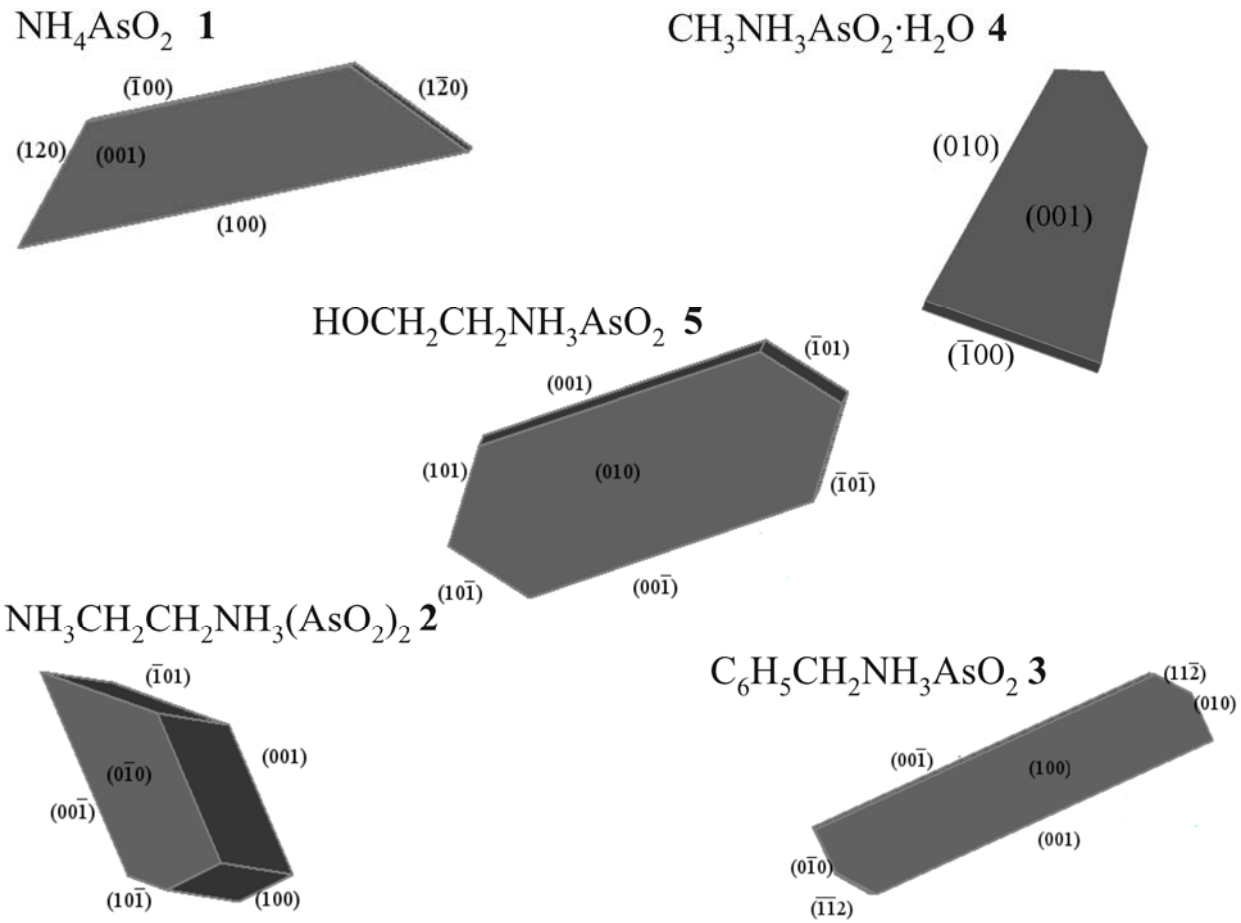

Fig. S1 Morphology of the obtained crystals of compounds **1-5**.

The greatest dimension of crystals of compounds **1-5** is parallel to the direction of primary structure's chains and the morphologically most important faces are parallel to the planes of secondary structure (Fig. S1). This is consistent with the PBC theory which states that the morphologically most important faces are parallel to at least two PBCs. In case of salts **2-5**

these PBCs are the anionic chain and the chain of hydrogen bonds connecting adjacent (AsO_2^-) chains in planes of the secondary structure. The habit of crystals of compound **1** is also consistent with the PBC theory predictions (Fig. S1). However, the morphologically most important face is not parallel to the planes of secondary structure. It is parallel to the PBC formed by the anionic chain and the PBC formed by the alternating N1−H3···O1^{iv} and N1−H4···O1^{v} hydrogen bonds (Fig. 3).

1. P. Hartman, in *Morphology of Crystals*, ed. I. Sunagawa, Terra Scientific Publishing Company (TERRAPUB), Tokyo, 1987, pp. 269-317