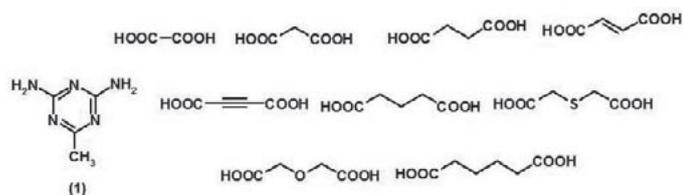


P09.02.20

Acta Cryst. (2008). A64, C480**pKa directed host-guest assemblies of 2,4-diamino-6-methyl-triazine with various dicarboxylic acids**Amit Delori¹, V. R. Pedireddi²¹National Chemical Laboratory, Division of organic chemistry, a.delori@ncl.res.in, Pune, Maharashtra, 411008, India, ²National Chemical Laboratory, vr.pedireddi@ncl.res.in, Pune, Maharashtra, 411008, India, E-mail: a.delori@ncl.res.in

Supramolecular synthesis by co-crystallization of compounds having complimentary functional groups is the general process of obtaining exotic targeted assemblies. Of particular interest are the complexes formed by aza-donor compounds like triazines, pyrimidines, etc., with compounds possessing functionalities such as -COOH, amides, cyclic imides, etc. In this direction, we have initiated studies with co-crystallization of 2,4-diamino-6-methyl-triazine, **1**, with various aliphatic dicarboxylic acids that differ by methylene or analogous groups, as shown in Scheme 1. These complexes were analyzed by single crystal x-ray diffraction studies to evaluate the structures in terms of recognition patterns, packing in three-dimensional arrangement, etc. All the complexes serve as representative examples in the class of host-guest assemblies, with two types of host networks being observed and differences are attributed to the variations in the pKa of the acid molecules under consideration, depending upon whether the pKa is above or below 3.0.



Keywords: pKa, host-guest complexes, supramolecular chemistry

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Acta Cryst. (2008). A64, C480**Cyclic transformation in novel shape and phase of C₆₀ nano/microcrystals**Akito Masuhara¹, Zhenquan Tan¹, Hitoshi Kasai^{1,2}, Hachiro Nakanishi¹, Hidetoshi Oikawa¹¹Tohoku University, Institute of Multidisciplinary for Advanced Materials, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan, ²PRESTO, Japan Science and Technology Agency (JST), 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan., E-mail: masuhara@tagen.tohoku.ac.jp

Fullerene C₆₀ has unique physical and electronic properties, and shows great potential in applications. To realize its potential applications, the preparation of well-defined low-dimensional nanostructures, i.e., C₆₀ nano/microcrystals (N/MCs) has been very important, and of much interest. But despite of these investigations, the size and shape control of C₆₀ N/MCs is still much difficult and a great challenge for scientists. Here, we would like to report the first time fabrication method of C₆₀ N/MCs having various shapes and a cyclic transformation in shapes and phases of solvent-participated C₆₀ N/MCs by exchanging the dispersion medium under supersonic irradiation: as-grown rod, disc, belt, rod, again. C₆₀ rod as a starting material of cyclic transformation was first fabricated from m-xylene / 2-propanol system by the SPRP (solvent-participated

reprecipitation process) [1] which was the improved technique of ordinary reprecipitation method [2]. Afterwards, C₆₀ rod were filtrated, redispersed again into 10 ml of ethanol, and then irradiated by supersonic for 2 hours. As a result, C₆₀ rod is changed to hexagonal disc. The similar procedures were repeatedly performed to further change the shape and phase of C₆₀ N/MCs. The phase transformation of C₆₀ N/MCs is due to the weak van der Waals interaction, while the resulting shape of C₆₀ N/MCs is dependent on the equilibrium form in a dispersion medium. These results provide the possibilities to well control the dimension and nanostructure of C₆₀ N/MCs for their great potential in nanodevices applications as well as to understand basically nanocrystallization process in molecular crystal solvates.

[1] Z. Tan A. Masuhara et al., *Jpn. J. Appl. Phys.* 47, 1426 (2008)[2] H. Kasai et al., *Jpn. J. Appl. Phys.* 31, L1132 (1992)

Keywords: nanocrystals, nanostructures, fullerenes

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Acta Cryst. (2008). A64, C480**Polymeric complex obtained from a novel supramolecular proton transfer compound**Shabnam Sheshmani¹, Mohammad Ghadermazi², Hossein Aghabozorg³¹Islamic Azad University, Shahr-e Rey Branch, Chemistry, Department of Chemistry, Islamic Azad University, Shahr-e Rey Branch, Qom Ave., Jihad Square, P. O. Box 18735-334, Tehran, Iran, ²Department of Chemistry, Kurdistan University, Sanandaj, Iran, ³Faculty of Chemistry, Teacher Training University, Tehran, Iran, E-mail: shabnam_sheshmani@yahoo.com

In this research, a novel supramolecular proton transfer compound was obtained from the reaction between pyridine-2,6-dicarboxylic acid, pydcH₂, and piperazine, pipz. According to the crystal structure, the proton transfer compound formulated as (pipzH₂)_{1.5}(pydcH)₃·3.7H₂O. This compound crystallizes in the space group C2/c of the monoclinic system and contains eight molecules per unit cell. The unit cell dimensions are: *a*=16.9584(9) Å, *b*=13.4081(7) Å, *c*=27.2449(2) Å and *β*=94.2140(1)°. The final *R* value was 0.0448 for 5573 reflections. One of two cations occupies a special position on inversion center. Also, one of water molecules occupies a special position on two-fold axis. All NH₂ groups of the cation molecules form with anion molecules the hydrogen bonds as type bifurcate N-H...O and N-H...N. In the crystal structure, hydrogen pyridine-2,6-carboxylate ions, (pydcH) are connected *via* hydrogen bonds as zigzag chains. Therefore, the intermolecular forces between cationic and anionic units in this compound consist of ion-pairing, hydrogen bonds and *π-π* stacking. Hydrogen bonds play a role in the construction of the supramolecular crystal structure. To an aqueous solution of proton transfer compound (pipzH₂)_{1.5}(pydcH)₃·3.7H₂O, was added a solution of Sr(NO₃)₂ in 2:1 molar ratio. The resulting complex crystallized in the monoclinic system with space group P2₁/c and contains four molecules per unit cell. The unit cell parameters are *a*=11.995(2) Å, *b*=13.701(2) Å, *c*=15.143(2) Å and *β*=90.098(3)°. The final *R* value was 0.0593 for 3936 reflections. The molecular structure of this complex is built of polymeric units of (pipzH₂) [Sr(pydc)₂(H₂O)₂].4H₂O, in which each pyridine-2,6-dicarboxylate moiety has acted as a tridentate ligand. Polymeric chains are connected by hydrogen bonds.

Keywords: supramolecular structures, polymeric materials, crystal structures