

## P06.06.17

*Acta Cryst.* (2008). A64, C388**Guest-induced topological polymorphism of pseudo-cubic hydrogen bond networks**

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Polymorphism has been the focus of constant attention, especially in the area of crystal engineering and pharmaceutical chemistry. Most of the polymorphic crystals were found by chance and still remain uninterpreted in detail, despite lengthy research. On the other hand, guest-inclusion and co-crystallization are recognized as standard tactics for obtaining different molecular arrangements. In fact, a great deal of inclusion crystals exhibit a wide variety of the guest-dependent arrangements of the host molecules. For control of the molecular arrangements, the concept of supramolecular synthon has been employed as one of the most influential concepts in the field of crystal engineering during the past decade. Up to now, many supramolecular synthons have been reported and applied to crystal design. Among them, finite and closed hydrogen bonds have been under intense study. An interesting supramolecular synthon involves a robust pseudo-cubic network due to twelve charge-assisted hydrogen bonds. In this report, we demonstrate the first example of the guest-induced topological polymorphism of the pseudo-cubic supramolecular synthons composed of primary ammonium carboxylates. The guest-inclusion caused a change in their crystal systems and a topological change of only one hydrogen bond of the synthons.

Keywords: topology, polymorphism, clusters

## P06.06.18

*Acta Cryst.* (2008). A64, C388**Supramolecular clusters composed of triphenylmethylamine and various sulfonic acids**

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Organic nanoparticles have attracted considerable research interest in molecular biology and life sciences as well as nanotechnology and materials science because of their unique properties. However, the preparation of nanoparticles with a uniform size has remained an important area of study. Furthermore, we can prepare homogeneously sized particles more efficiently and in greater amounts by borrowing techniques from supramolecular chemistry. With respect to supramolecular clusters, we have studied [4+4]-type clusters, which consist of eight organic components of two types connected through hydrogen bonds. We recently described the self-assembly of four ammonium and four triphenylacetate ions into a [4+4] ion-pair cluster through a cubic network of hydrogen bonds. However, these clusters are obtained only in a few combinations of amines and triphenylacetate. In this report, we describe that [4+4] ion-pair clusters composed of triphenylmethylammonium and sulfonate ions can be obtained easily and efficiently in the solid state and in solution with many different sulfonic acid derivatives. The universality of sulfonate-containing clusters, as observed in these experiments, contributes to their potential utility. These novel clusters have

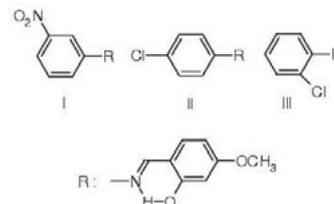
inherent shapes and sizes that are controlled by the substituent on the sulfonic acid. Their preparation is based on the specificity of the combination of the ammonium and sulfonate ions; this system is potentially useful for synthesizing organic nanoparticles.

Keywords: supramolecular cluster, cubic network, hydrogen bond

## P06.10.19

*Acta Cryst.* (2008). A64, C388**Crystal structure and *ab initio* calculations of three 4-methoxy salicylaldehyde derivatives**Orhan Buyukgungor<sup>1</sup>, Basak Kosar<sup>1</sup>, Cigdem Albayrak<sup>2</sup>, Mustafa Odabasoglu<sup>2</sup><sup>1</sup>Ondokuz Mayıs University, Physics Department, Kurupelit, Samsun, TR-55139, Turkey, <sup>2</sup>Ondokuz Mayıs University, Chemistry Department, Kurupelit, Samsun, TR-55139, Turkey, E-mail: orhanb@omu.edu.tr

Schiff bases are widely used as ligands in the field of coordination chemistry and they play an important role in various field of chemistry due to their biological activities [1]. Here we report the molecular and crystal structures of (*E*)-5-Methoxy-2-[(3-nitrophenylimino) methyl]phenol, (*E*)-2-[(4-chlorophenyl imino) methyl]-5-methoxyphenol and (*E*)-2-[(2-chlorophenylimino) methyl]-5-methoxyphenol labeled as I, II and III, respectively. The optimized molecular geometries and energies of I, II and III were calculated using the restricted Hartree-Fock with 6-31+G(d,p) basis set. In the solid state, compounds adopt the enol-imine tautomeric form with the H atom located on O rather than N. In the optimized geometry, the total energies of molecules are -945.41, -1200.83 and -1200.82 Hartrees for I, II and III, respectively.

[1] Lozier, R.; Bogomolni, R. A.; Stoekenius, W. J. *Biophys.* 1975, 15, 955.Keywords: schiff bases, enol-imine, *ab initio*

## P06.06.20

*Acta Cryst.* (2008). A64, C388-389**Constructions of higher order architectures by connecting of 4+4 supramolecular clusters**

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Hydrogen-bonded supramolecular synthons represent effective tools for crystal engineering. Recently, we have reported that organic salts composed of four triphenylacetic acids and four amines construct a cluster like a cubane through hydrogen bonds. Moreover, we succeeded in forming clusters with triphenylmethylammonium monosulfonates (Fig.1), which possess discrete hydrogen-bonded networks, and shape such as a tetrapod. Surprisingly, a wide range of sulfonic acids yield the clusters without exception. Here we show a connection of the supramolecular clusters with ammonium disulfonates. The connection has three kinds of networks. The first is 4-fold diamondoid network. The crystals have large channel-type spaces where various organic molecules are included. The next is