$LiBD_4$ and $LiNH_2$ precursors. To avoid the high absorption of natural boron, pure $^{11}B$ was used. The isotopically labeled, mixed H/D sample enabled the determination of D/H occupancies on the four distinct sites. The structure was analysed by Rietveld refinement, proving the space group and revealing H-N-N and D-B-D bond angles and metal – hydrogen atomic distances.

[1] Hoelzel M., Senyshyn A., Gilles R., Boysen H., Fuess H. *Neutron News* 18(4) **2007**.

**Keywords: hydrogen storage; hydride structure; neutron diffraction**

## FA2-MS04-P10

**Kinetic and Morphological Effects of Biopolymers on the Growth of Hydroxyapatite Crystals.** Özlem Doğan[a], Özge Cinel[a], Mualla Öner[a]. [a]*Yıldız Technical University, Chemical Engineering Department, Davutpasa 34210 Istanbul, Turkey.*
E-mail: dogano@yildiz.edu.tr

Modelling of the biologic materials require crystallization strategies that provide control over the structure, size and morphology of inorganic crystals. The biological synthesis of inorganic solids often yields materials of uniform size, unusual habit, organized texture and defined structure and composition under moderate conditions of supersaturation and temperature (1, 2). Additives of both organic and inorganic nature play an important role in crystallization processes. They alter the surface properties of the crystals which leads to changes in nucleation and growth (3). The growth of nuclei is affected by adsorption these molecules on the active growth sites (4).
In the present work, the effect of a polysaccharide-based polycarboxylate biopolymers on the crystal growth kinetics of hydroxyapatite was studied by seeding stable supersaturated calcium phosphate solutions with crystals. Carboxymethyl inulin which has a three different number of carboxylate group has been used as additive. The polymer concentration and the carboxylation degree of the polymer were important factors for controlling crystallization.

[1] Öner M., Doğan Ö., *Progress in Crystal Growth and Characterization of Materials,* **2005**, 50, 39. [2] Nancollas G.H., Wu W., *J.Crystal Growth* 211, **2000**,137. [3] Öner M., Doğan Ö., Öner G., *J.Crystal Growth,* **1998**, 186, 427. [4] Lioliou M.G., Paraskeva C.A., Koutsoukos P.G., Payatakes A.C., *J.Colloid and Interface Science*, **2006**, 303, 164.

**Keywords: hydroxyapatite; biopolymers; crystallization**

## FA2-MS04-P11

**Control of Calcium Oxalate Crystallization by Using Polymeric Additives.** Emel Akyol[a], Semra Kırboğa[a], Mualla Öner[a]. [a]*Department of ChemicalEngineering, Yıldız Technical University, İstanbul, Turkey.*
E-mail: eakyol@yildiz.edu.tr

Chemical Engineers and urologists have been interested in calcium oxalate crystallization for many years due to its importance on biomineralization and industrial crystallization applications [1,2]. Calcium oxalates are the main components of both pathological deposits in the urinary tract and scale formed on the radiator tubes in evaparators [3,4]. Deposits are desired to remove from the solution in industrial applications since they may reduce the heat transfer efficiency. One common method to inhibit the scale formation is using a suitable additive.
In this study, the effects of acrylic acid and vinylsulfonic acid copolymers on the growth mechanism of the calcium oxalate crystals have been investigated by using spontaneous crystallization method. All polymers tested in this study are effective as growth inhibitors under the experimental conditions. Some of copolymers not only provided the inhibition of calcium oxalate crystallization but also changed the crystal morphology.

[1] Zauner R., Jones A. G., *Ind. Eng. Chem. Res*., **2000**, 39, 2392. [2] Bertherton T., Rodgers A., *Journal of Crystal Growth*, **1998**, 192, 448. [3] Akyol E., Öner M., *Journal of Crystal Growth*, **2007**, 307, 137. [4] Thongboonkerd V., Semangoen T., Chutipongtanate S., *Clinica Chimica Acta*, **2006**, 367, 120.

**Keywords: calcium oxalate; additive; crystallization**

## FA2-MS04-P12

**The Phenyl Substitution Effects on the 2,4,6-Triphenoxy-1,3,5-Triazines.** Alajos Kálmán[a], Petra Bombicz[a], Nikoletta B. Báthori[a]. [a]*Institute of Structural Chemistry, Chemical Research Center, HAS, Budapest, Hungary.*
E-mail: akalman@chemres.hu

Semirigid molecules [1] easily form isostructural [2] groups which may then be related via morphotropic steps [3] *i.e.* by virtual non-crystallographic rotations (*ncr*) and/or translations (*nct*) [4]. Occasionally, polymorphs are also formed from isostructural layers or columns [5] via morphotropism. The semirigid molecules of the title compounds [6] prompted us to study the links between their isostructural groups [7]. Revisiting [8] the supramolecular symmetries disclosed for the Piedfort Units (PUs) [9], now we compare the effects of aryl substitution: i) how do the *ortho, meta* or *para* functions influence the perfect or relaxed $C_3$ molecular symmetry and ii) what are the common motives of these structures linked by virtual *ncr*-s and/or *nct*-s.
The *para*-substitutions restore the $C_3$ axis relaxed in the parent molecule (POT) which crystallizes in space group *Ia*. The columns of the 4-XPOT derivatives are held together by three parallel glide planes in space group $R3c$. Isostructurality of the alkyl row is terminated by the $^t$Butyl functions. One of the aryl groups rotates through 180° around the O-C(triazine) bond and the molecules crystallize in space group $P2_1/c$ [10]. The smallest *halo* function F retains the relaxed $C_3$ symmetry of POT, but every second band of the molecules rotates around the *b* axis by 180°. The glide planes of *Ia* at $y = \pm¼$ are converted into centers of inversion in space group $P2_1/c$. Thus POT and 4-FPOT