

LiBD<sub>4</sub> and LiNH<sub>2</sub> precursors. To avoid the high absorption of natural boron, pure <sup>11</sup>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.

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

#### FA2-MS04-P10

**Kinetic and Morphological Effects of Biopolymers on the Growth of Hydroxyapatite Crystals.** Özlem Doğan<sup>a</sup>, Özge Cinel<sup>a</sup>, Mualla Öner<sup>a</sup>. <sup>a</sup>*Yıldız Technical University, Chemical Engineering Department, Davutpasa 34210 Istanbul, Turkey.*

E-mail: [dogano@yildiz.edu.tr](mailto: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.

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**Keywords: hydroxyapatite; biopolymers; crystallization**

#### FA2-MS04-P11

**Control of Calcium Oxalate Crystallization by Using Polymeric Additives.** Emel Akyol<sup>a</sup>, Semra Kirboğa<sup>a</sup>, Mualla Öner<sup>a</sup>. <sup>a</sup>*Department of Chemical Engineering, Yıldız Technical University, İstanbul, Turkey.*

E-mail: [ekayol@yildiz.edu.tr](mailto:ekayol@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 evaporators [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.

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

#### FA2-MS04-P12

**The Phenyl Substitution Effects on the 2,4,6-Triphenoxy-1,3,5-Triazines.** Alajos Kálmán<sup>a</sup>, Petra Bombicz<sup>a</sup>, Nikolett B. Báthori<sup>a</sup>. <sup>a</sup>*Institute of Structural Chemistry, Chemical Research Center, HAS, Budapest, Hungary.*

E-mail: [akalman@chemres.hu](mailto: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<sub>3</sub> 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<sub>3</sub> 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 'Butyl' functions. One of the aryl groups rotates through 180° around the O-C(triazine) bond and the molecules crystallize in space group *P2<sub>1</sub>/c* [10]. The smallest *halo* function *F* retains the relaxed C<sub>3</sub> symmetry of POT, but every second band of the molecules rotates around the *b* axis by 180°. The glide planes of *Ia* at *y* = ±¼ are converted into centers of inversion in space group *P2<sub>1</sub>/c*. Thus POT and 4-FPOT

show 2D-isostructurality.

The *meta*-substitutions, except 3-IPOT (*R*-3), lead to space group *P*-3*c*1. However, in both stacking forms  $C_{3i}$ -PU<sup>endo</sup> is common. It denotes PUs in which there is a crown formed by six *halo* atoms. They are separated by centers of inversion in 3-IPOT forming  $C_{3i}$ -PU<sup>exo</sup>-s, while in 3-BrPOT *etc.* every second diad turns upside down along the -3 axis. Thus  $D_3$ -PUs are formed between the  $C_{3i}$ -PU<sup>endo</sup>-s. As a whole, the *odd* and the *even* layers are separately isostructural.

The repulsion between the *ortho*-functions (F->I) modelled in 3-IPOT separates the  $C_{3i}$ -PU<sup>exo</sup>-s and shifts them by *ca* 4.8 Å perpendicular to the former molecular column. These *nct*-s invariably result in triclinic unit cells [6]. While in 2-FPOT it contains one PU<sup>exo</sup> with relaxed  $C_{3i}$  symmetry, in the unit cells of 2-Cl/Br/IPOTs there are two diads. In the isostructural 2-BrPOT and 2-IPOT every second row of the diads rotates *ca* 90°, while in 2-CIPOT this rotation is only about 47° [10].

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**Keywords:** isostructurality; morphotropism

#### FA2-MS04-P13

**Crystal Structure of  $Na_3MgTi(PO_4)_3$ ,** Saïda Krimi<sup>a</sup>, Abdelaziz El Jazouli<sup>b</sup>, ETA. Lachgar<sup>c</sup>. <sup>a</sup>LPCMI, Faculté des Sciences Ain Chock, Casablanca, Maroc. <sup>b</sup>LCMS, Faculté des Sciences Ben M'Sik, Casablanca, Maroc. <sup>c</sup>Department of Chemistry, Wake forest University, Winston-Salem, North Carolina 27109, USA.  
E-mail: [krimisaida@yahoo.fr](mailto:krimisaida@yahoo.fr)

Sodium titanium phosphates have been studied in the context of various fields of solid state chemistry : low thermal expansion ceramics [1], electrode materials [2], solids electrolytes [3]. In course of the investigation of the phase diagram for four component systems  $Na_2O - MgO - TiO_2 - P_2O_5$ , we have isolated the new titanium phosphate  $Na_3MgTi(PO_4)_3$  [4]. Growth of single crystals allowed us to determine the structure and describe in this present paper. Single crystals samples of  $Na_3MgTi(PO_4)_3$  were prepared using  $Na_2CO_3$ ,  $MgCO_3$  carbonates,  $TiO_2$  oxide and  $(NH_4)_2HPO_4$  phosphate in stoichiometric amounts. The single crystals were grown from the melt. In the platinum crucible the mixture are first heated at 473(12hr), 673(4hr) and 973 (12hr). It are then heated to 1173K and held at this temperature for 20 mn, cooled to 773K at the rate of 5°C/hr and finally furnace cooled to room temperature. The crystals obtained are transparent, colourless and enclosed in rectangular parallelepiped.

The  $Na_3MgTi(PO_4)_3$  are at 293°K, trigonal and belongs to space group  $R\bar{3}$  ( $Z = 6$ ) with the hexagonal cell parameters :  $a_h = 8.792(2)$  Å,  $c_h = 22.039(3)$  Å,  $d_{exp} = 2.91(2)$  and  $d_{cal} = 2.88$ . The resulting structural parameters have been refined to convergence [ $R_1 = 0.025$  and  $wR_2 = 0.073$ ] using counter – weighted full – matrix least – squares techniques and a structural model which incorporated anisotropic thermal parameters for all atoms.

The structure of  $Na_3MgTi(PO_4)_3$ , belongs to the Nasicon –type family, consist of three dimensional network of  $PO_4$  tetrahedra and  $AO_6$  [ $A \equiv Ti, Mg$ ] octahedra sharing corners. These octahedra are occupied successively by the titanium and magnesium atoms along the *c* axis. The structure contains two different sites labelled M(1). One of the two M(1) site positions (3b : 0,0,1/2) is totally occupied by sodium atoms Na(1) shares common faces with two  $MgO_6$  octahedra. Whereas the other site position (3a : 0,0,0) is partially occupied by Na(2) neighboring two  $TiO_6$  octahedra. The cationic ordering giving rise to infinite chains parallel to the [001] direction with following distribution :  $[TiO_6][MgO_6][Na(1)O_6][MgO_6][TiO_6][Na(2)O_6][TiO_6][MgO_6]$  The remaining sodium atoms are located in the larges cavities labelled M2 site.

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**Keywords:** titanium phosphates; nasicon type

#### FA2-MS04-P14

**Absorption X-Ray in Quartz Crystal with Temperature Gradient.** Vahan R. Kocharyan. *Institute of Applied Problems of Physics, National Academy of Sciences, Republic of Armenia.*  
E-mail: [vahan2@yandex.ru](mailto:vahan2@yandex.ru)

Discovery of the phenomenon of complete transfer of X-rays from the direction of passage to the reflection direction in Laue geometry [1] at  $\mu t > 1$  ( $t$  is the thickness of the crystal and  $\mu$  is the coefficient of the linear absorption) was the powerful contribution to the development of x-ray optics. The behavior of the linear absorption of X-rays in a quartz single crystals on Laue geometry is experimentally studied in [2,3]. It has been shown that the presence of the temperature gradient [2] and the ultrasonic vibrations [3] leads to essential reduction of absorption of X-rays (in case of ultrasonic vibrations up to nulling). In the present work the theoretical analysis of the mentioned process in plane wave approximation in presence of a temperature gradient is carried out. The Takagi's equations, describing propagation of the wave field in deformed crystal are analytically solved [4]. The deformation field of a crystal is chosen in the form of  $U_x = (t^2 - (t - 2z)^2) / 8R$ , where  $R$  is the radius of curvature of reflecting atomic planes,  $x$  axis is directed parallel to the diffraction vector, and  $z$  axis is directed parallel to the normal of a surface of a crystal. The theoretical analysis shows that (with beam penetration in a crystal) the presence