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^{6endo} 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^{6exo}-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^{6endo}-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^{6exo}-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^{6exo} 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-ClPOT this rotation is only about 47° [10].
The work was supported by Hungarian Research Fund (OTKA) T049712.

[1] Kálmán, A, Fábián, L. *ActaCryst.* **2007**, B63, 411; [2] Fábián, L., Kálmán, A. *ActaCryst.* **1999**, B49, 1039; [3] Kitaigorodskii, A.I. *Organic Chemical Crystallography*, Consultants Bureau, N.Y., 1961; [4] Kálmán, A. *ActaCryst.* **2005**, B61, 536; [5] Fábián, L., Kálmán, A. *ActaCryst.* 2004, B60, 547; [6] Saha, B.K., Nangia, A. *Heteroatom Chem*. **2007**, 18, 185 and refs therein; [7] Kálmán, A., Bombicz, P. *ActaCryst.* **2007**, A63 s202; [8] Bombicz P., Kálmán, A. *Cryst. Growth Des*. **2008**, 8, 2821; [9] Thalladi, V.R. *et al., J.Am.Chem.Soc.* **1998**, 120, 2563; [10] Báthori, N.B. *PhD Thesis,* Budapest, **2006**.

Keywords: isostructurality; morphotropism

FA2-MS04-P13

Crystal Structure of $Na_3MgTi(PO_4)_3$. Saïda Krimi[a], Abdelaziz El Jazouli[b], ETA. Lachgar[c]. [a]*LPCMI, Faculté des Sciences Aïn Chock, Casablanca, Maroc.* [b]*LCMS, Faculté des Sciences Ben M'Sik, Casablanca, Marocc.* [c]*Department of Chemistry, Wake forest University, Winston-Salem, North Carolina 27109, USA.*
E-mail: 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, dexp = 2.91(2) and dcal = 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 ≡ 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.

[1] Barth, S. And al. Mater. Lett., 16(Issues 2-3), 96-101, **1993**. [2] Aatiq, A., and al. *J. Solid State Chem*., 174, 158-169, **2001**. [3] Hasegawa, Y. And al. J. Alloys Comp., 375, 212-216, **2004**. [4] Krimi S. and al phosphorus Research Bulletin, 15, 155-158 , **2004**.

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

Discovery of the phenomenon of complete transfer of X-rays from the direction of passage to the reflection direction in Laue geometry [1] at μt>1 (t is the thickness of the crystal and μ 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 Ux=(t2-(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