

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-ClPOT 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.  
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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 largest 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.*  
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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

of the curvature leads to the increasing of the amplitude of the diffracted and weakly absorbed field and simultaneous decreasing of the amplitudes of diffracted and strongly absorbed field as well as amplitude of both passing fields. With increasing the curvature of the reflecting atomic planes, the energy transferred to the diffracted weakly absorbed field is increases. There is a certain value of the curvature for which the total energy is transmitted only to this field. As a consequence the absorption coefficient of the crystal is sufficiently decreases. The further increasing of the curvature leads to decreasing of the energy transferred to the diffracted weakly absorbed field (the absorption coefficient is increased again). In order to explain the above-mentioned processes the total intensity of passed and diffracted beams in the region of Darwin's table are analysed at different curvatures of reflecting atomic planes. It is shown that with decreasing the radius of curvature the total intensity at exactly Bragg angle and over all region of Darwin's table is increased, i.e. the absorption coefficient is decreases. Theoretical calculations have been carried out for a quartz single crystal for several families of reflecting atomic planes. However the above-mentioned effect was most obviously manifested for (10-11) family of reflecting planes.

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**Keywords: X-ray diffraction; external influences; linear absorption coefficient**

#### FA2-MS04-P15

#### Crystallography of CuZnAl Austenite via Combined XANES, EXAFS and XRD Analysis.

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Shape memory alloys (SMAs) belong to the class of smart materials (together with ferroelectric, piezoelectric, etc.) since they underscore a reversible variation in macroscopic size driven by changes of external conditions (temperature, pressure, or magnetic field). SMAs can be as consequence employed in the manufactory of actuators controlled by one of these external parameters and, viceversa, in the design of sensors. SMAs have several applications in the field of engineering and medical science: tube coupling, active endoscopes, and artificial muscle components for robotics. The shape memory behavior is due to a displacive phase transition (martensitic) which takes place in different metals. This transformation is a cooperative phenomenon (like

ferromagnetism) which, despite the small displacement of the single atoms, results in a macroscopic shape variation since all atoms move in the same direction into a domain. We have investigated and solved the structure of the parent phase (austenite) of the martensitic transition in CuZnAl shape memory alloys by a combined X-ray absorption (EXAFS, XANES) and diffraction analysis [1], taking advantage of the different length scale sensitivity of the two techniques. Ab-initio simulations of the near Zn-edge X-ray absorption coefficient (XANES) allow us to directly discard the hypothesis of a DO<sub>3</sub> superstructure. At the same time, we give evidence of the existence of an ordered structure (B2-like) different from the L2<sub>1</sub>, one recently proposed by neutron diffraction [2]. However, some partial L2<sub>1</sub> ordering is present at room temperature: this superstructure develops and recovers order when increasing the temperature above 400 K. Note that DO<sub>3</sub> and L2<sub>1</sub> phases differ only for the relative site occupancy by Zn and Cu atoms, indeed they cannot be discriminated by the sole X-ray diffraction, due to the close atomic number of the two elements. The formation of either B2-like or L2<sub>1</sub> superstructures has an important effect on the martensitic transition temperature. Our work presents a typical example in which X-ray Absorption can be used for crystallographic phase determination when the very similar X-ray scattering factors of the elements present in the alloy makes some ordering configurations invisible to X-ray diffraction only. The same method can be applied in the study of other intermetallic compounds.

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