appear at 1416 and 1609 $cm^{-1}$ characteristic respectively to symmetric and anti-symmetric vibration of COO- of tartaric acid. The intensity of COO- bands increases as function of acid concentration in solution and with zinc content, implying the formation of calcium and zinc tartarate on the hydroxyapatite surface. The NMR-MAS $^{13}C$ spectra of hydroxyapatite treated present two peaks at 74 and 181 ppm characteristic of two different carbons of tartaric acid. The formation of new hybrid coumpounds was confirmed by the shift of signals comparing with those of free tartaric acid. Moreover, the broadening of these peaks can be explained by the heterogeneity of carbon environment by the presence of zinc on the apatitic surface.

[1] T. Turki, A. Aissa, H. Agougui, M. Debbabi, *journal de la société chimique de tunisie*, **2010**, *12*, 161-172.

**Keywords: apatite, surface, fonctionnel**

## MS74.P16

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**How to deal with multiple solutions in powder pattern indexing**

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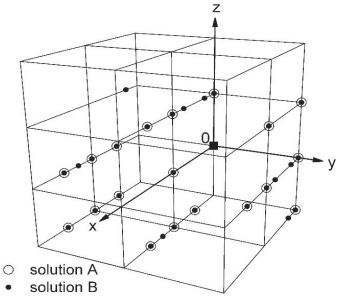
Santoro et al (1980) [1] first addressed the question of equivalence when in powder pattern indexing more than one indexing solution and thus more than one reciprocal metric tensor are produced. Two metric tensors $G^*_A$ and $G^*_B$ are said to be equivalent when a matrix R exists such that $G^*_B = RG^*_A R^T$ (1). R is a $3\times3$ non-symmetric matrix consisting of rational numbers. Therefore, eq. (1) cannot be solved directly. Santoro et al (1980) [1] suggested to vary the elements of R systematically in the range (5, -5) until the equality sign in eq. (1) is fulfilled within chosen error limits.

We suggest a different procedure: First, the three shortest non-coplanar vectors that have the same Q values in both lattices A and B are identified. These vectors are taken to define a new basis common to A and B. Then, $3\times3$ matrices $M_A$ and $M_B$ are written which transform the axial systems of A and B into the new one. If the new axial system reproduces lattices A and B, then the equality $M_A G^*_A M^T_A = M_B G^*_B M^T_B$ (2) holds. Eq. (2) defines a new metric tensor common to both lattices A and B which we thus term the common metric tensor $G^*_C$. The coordinates of the reciprocal lattice points of A and B are transformed according to $(\eta/\kappa/\lambda)_{A,B} = (M^{-1}_{A,B})^T (h/k/l)_{A,B}$. Coincident lattice points yield $(\eta/\kappa/\lambda)_A = (\eta/\kappa/\lambda)_B$. If all lattice points coincide, lattices A and B are termed equivalent; if only a subset of points is coincident, the lattices are semi-equivalent; otherwise they are non-equivalent.

Equation (1) can be easily retrieved from equation (2): $G^*_B = M^{-1}_B M_A G^*_A M^T_A (M^{-1}_B)^T = RG^*_A R^T$. Thereby we arrive at a solution to eq. (1) that avoids trial and error methods.

We take as an example two different indexing solutions A and B to $CrPO_4.6H_2O$, given by Santoro et al. (1980) [1], to demonstrate the spatial relationship of the respective reciprocal lattice points. Fig. 1 shows that lattice points A and B coincide. However, solution A only explains a subset of points.




[1] A. Santoro, A.D. Mighell, J.R. Rodgers, *Acta Cryst.* **1980,** *A36,* 796-800.

**Keywords: powder pattern indexing, multiple solutions, metric tensor**

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**XRD and SAXS studies applied to doped Polyaniline and Poly(*o*-methoxyaniline)**

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Polyaniline (PANI) and derivatives of aniline have received great attention due to their technological applications. The introduction of polar functional groups and alkyl groups to the main chain of PANI is a practice to obtain soluble polymers in a wider variety of organic solvents. Poly(*o*-methoxyaniline) (POMA) is a derivative of PANI and its structural difference is the presence of the group ($-OCH_3$) in the *ortho* position of the carbon rings, been extensively studied in the form of powder or films for the most various applications. ES-PANI and ES-POMA were synthesized, respectively, according to the method described elsewhere [1,2] with times of synthesis ranging from 0,5 to 96 h. Samples were characterized by XRD, SAXS, LeBail Fit [3], SEM and van der Pauw method [4]. XRD analysis showed that the synthesis time was not significant in the crystallinity of PANI, however, it is an important parameter in the synthesis of POMA, which became more crystalline. LeBail Fit showed that the ES-PANI crystallites average size is 34 Å, while for ES-POMA the crystallites average size increases with increasing synthesis time (from 26 to 57 Å). By SAXS it was possible to obtain values of Radius of Giration ($R_g$) (217Å for ES-PANI and 280 – 313Å for ES-POMA); the maximum particle size ($D_{max}$) from the Pair-distance distribution Function ($p(r)$) (650Å for ES-PANI and 900Å for ES-POMA) and the particle organization qualitative analysis through Kratky curves, showing that for ES-PANI the crystallinity does not increase significantly over synthesis; for ES-POMA, particles became more ordered with increasing of crystallinity over the synthesis. Images of SEM allowed the visualization of different morphologies for PANI and POMA: while the PANI-ES showed fiber morphology formed by interconnected nanospheres, the POMA-ES had a globular vesicular morphology, which changed with increasing synthesis time. Conductivity measurements were not changed drastically in different synthesis time for ES-PANI ($1{,}84.10^{-4}$S/cm), whereas for the ES-POMA the conductivity increased during the synthesis ($1{,}89.10^{-7}$ to $8{,}89.10^{-7}$S/cm). The results obtained by each of the techniques were essential to the understanding of the structure and properties of polymeric materials.

[1] S. Bhadra, N.K. Singha, D. Khastgir. *Journal of Applied Polymer Science* **2007**, *104*, 1900–1904.[2] J.M. Yeh, C.P. Chin. *Journal of Applied Polymer Science* **2003**, *88*, 1072–1080. [3] A. LeBail, H. Duroy, J.L. Fourquet. *Materials Research Bulletin* **1988**, *23*, 447–452. [4] R. Robert, S.M. Berleze, *Revista Brasileira de Ensino de Física* **2007**, *29*, 15-18.

**Keywords: polyaniline, poly(o-methoxyaniline), XRD**

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**The magnetic ordering in $Mn_3TeO_6$ and $Co_3TeO_6$**

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