SYNTHESIS AND STRUCTURAL COMPARISON BETWEEN
Ag$_2$SnFe(PO$_4$)$_3$ and Na$_{1.5}$X$_{1.5}$Sb$_{0.3}$(PO$_4$)$_3$ (X = Ti, Sn)

PHOSPHATES

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Phosphates within the Nasicon-type family have been the subject of intensive research due to their potential applications as a solid electrolyte, electrodes materials, low thermal expansion ceramics [1] and as storage materials for nuclear waste [2]. The crystal structure of A$_x$XX’(PO$_4$)$_3$ family is formed of corner-sharing X(X’)O$_6$ octahedra and PO$_4$ tetrahedra in such a way that each octahedron is surrounded by six tetrahedra and each tetrahedron is connected to four octahedra. These compounds crystallise mainly with the Nasicon Na$_2$Zr$_2$(PO$_4$)$_3$-type structure (R$\bar{3}$c space group) [3]. The A cation are generally located in the interconnected interstitial sites usually denoted M1 and M2 sites (crystallographic formula [M1][M2]$_3$XX’(PO$_4$)$_3$).

Recently, the structural characteristics by X-ray powder diffraction (XRD) study using the Rietveld method for K$_2$SnB(PO$_4$)$_3$ (B = Fe, Yb, In and Cr) phases were realised [4,5]. The four materials exhibit the Langbeinite-type structure. In a continuation of our search concerning phosphates with interesting physical applications, the principal objective of the present study was the structural determination, using Rietveld refinement of the XRD patterns, of the three newly synthesised Ag$_2$SnFe(PO$_4$)$_3$ and Na$_{1.5}$X$_{1.5}$Sb$_{0.3}$(PO$_4$)$_3$ (X = Ti, Sn) ceramics phosphates. The three compounds have been prepared by solid state reaction techniques. Their structures were determined at room temperature from (XRD) using the Rietveld analysis. Results of the structure refinement show that all materials exhibit the Nasicon-type structure. Ag$_2$SnFe(PO$_4$)$_3$ crystallises in the R-3c space group, and both Na$_{1.5}$X$_{1.5}$Sb$_{0.3}$(PO$_4$)$_3$ (X = Ti, Sn) phases crystallise in the R-3 space group. Hexagonal unit cell parameter values are: a = 8.676(1) Å and c = 22.498(1) Å for Ag$_2$SnFe(PO$_4$)$_3$, a = 8.460(1) Å and c = 21.835(1) Å for Na$_{1.5}$Ti$_{1.5}$Sb$_{0.3}$(PO$_4$)$_3$ and a = 8.457(1) Å and c = 22.472(1) Å for Na$_{1.5}$Sn$_{1.5}$Sb$_{0.3}$(PO$_4$)$_3$. The final Rietveld refinement lead to acceptable reliability factors. Close structural examination shows a partial occupancy of Ag$^+$ ions within the two available M1 and M2 sites of the Ag$_2$SnFe(PO$_4$)$_3$ Nasicon-structure. In both Na$_{1.5}$X$_{1.5}$Sb$_{0.3}$(PO$_4$)$_3$ (X = Ti, Sn) ceramics, all Sb$^{5+}$, X$^{4+}$ ions and 0.2 Na$^+$ occupied the Nasicon- framework, the other 1.3 Na$^+$ are distributed between the two M1 and M2 sites.
