

Structure and spectroscopic study of Nasicon phosphates series

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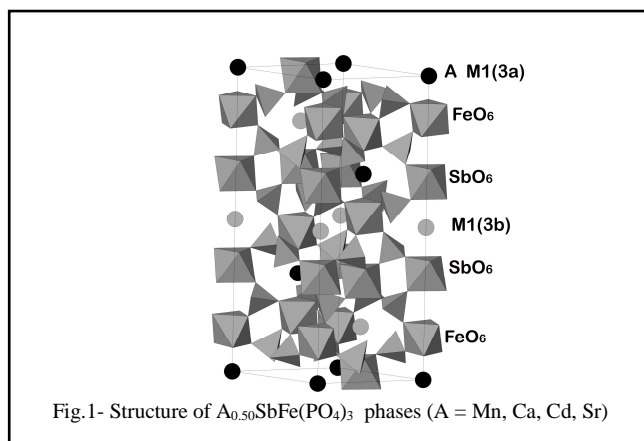
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Abstract:

The Nasicon-type family has been the subject of intensive research due to its potential applications as solid electrolyte, electrode material, low thermal expansion ceramics and as storage materials for nuclear waste [1-4]. The structure of such materials with general formula $A_xX'X''(PO_4)_3$ consists of a three-dimensional network made up 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 octahedral (Fig. 1). Within the Nasicon framework, there are interconnected interstitial sites usually labelled M1 (one per formula unit) and M2 (three per formula unit) through which A cation can diffuse, giving rise to a fast-ion conductivity. The crystallographic formula can be written as $[M1][M2]_3X'X''(PO_4)_3$.

Nasicon phosphates samples $A_{0.5}SbFe(PO_4)_3$ were obtained by solid state reaction in air. The structural characteristics by powder X-ray diffraction (XRD) study using the Rietveld method show that all compounds are isostructural and crystallise in the $R\bar{3}$ space group. In all samples, A^{2+} cations occupied one-half of the M1 sites and the Sb^{5+} and Fe^{3+} cations are orderly distributed within the $SbFe(PO_4)_3$ framework (Fig.1). A globally structural comparison between $A_{0.50}SbFe(PO_4)_3$ phases are presented. In order to obtain further structural information about the nature of bonding in studied phosphates an assignment of Raman and Infrared bands was also realised.



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