Crystal structure of lead dinickel iron tris(orthophosphate): $PbNi_2Fe(PO_4)_3$

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The new orthophosphate $PbNi_2Fe(PO_4)_3$ have been synthesized by solid-state reaction route and characterized by X-ray diffraction, scanning electron microscopy, Infrared and Raman spectroscopy.

The analysis by single crystal and powder X-ray diffraction techniques showed that this compound crystallizes in the orthorhombic system with Imma space group and unit cell parameters a = 10,415 (3) Å; b = 13,165 (4) Å; c = 6,536 (2) Å; V = 896,15 (5) $Å^3$; Z = 4.

The three-dimensional framework of the crystal structure is built up by $[PO_4]$ tetrahedra, $[FeO_6]$ octahedra and $[Ni_2O_{10}]$ dimers of edge-sharing octahedra, linked through common corners or edges. This structure comprises two types of layers stacked alternately along the [100] direction. The first layer is formed by edge sharing octahedra ($[Ni_2O_{10}]$ dimer) linked to $[PO_4]$ tetrahedra via common edges and vertices while the second layer is built up from a row of corner-sharing $[FeO_6]$ octahedra and $[PO_4]$ tetrahedra forming an infinite linear chain. The layers are held together through vertices of $[PO_4]$ tetrahedra and $[FeO_6]$ octahedra, leading to the appearance of two types of tunnels parallel to the a and b-axis directions in which the Pb^{2+} cations are located.

The structure affiliation of the studied phosphate to that of α-$CrPO_4$ and its spectroscopic properties will be discussed.

Keywords: X-ray diffraction; crystal structure; solid-state reaction; phosphate; α-$CrPO_4$