Crystal structure of lead dinickel iron tris(orthophosphate): PbNi$_2$Fe(PO$_4$)$_3$

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The new orthophosphate PbNi$_2$Fe(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$_2$O$_{10}$] 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$_2$O$_{10}$] 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$_4$