Synthesis, Crystal Structure, Ca^{2+} and Proton Conduction Pathways of New Triphosphate $\text{Ca}_{0.5}\text{FeHP}_3\text{O}_{10}$

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A new calcium iron phosphate $\text{Ca}_{0.5}\text{FeHP}_3\text{O}_{10}$ was synthesized under hydrothermal conditions at 453K and studied by single-crystal X-ray diffraction at room temperature. It crystallized in monoclinic space group $C2/c$ with lattice parameters $a = 12.102(3) \text{ \AA}$, $b = 8.459(2) \text{ \AA}$, $c = 9.387(3) \text{ \AA}$, $\beta = 112.21(2)^\circ$, $V = 889.7(4) \text{ \AA}^3$ and $Z = 4$. The final agreement factors are $R(F^2) = 0.027$ and $wR(F^2) = 0.073$. The anionic framework of the title compound consists of FeO_6 octahedra linked by hydrogentriphosphate HP_3O_{10} anions to form a three-dimensional framework containing tunnels parallel to c -axis where Ca^{2+} cations are located. The structural model was validated by bond valence sum (BVS), distortion indices (DI) and charge distribution (CD) methods. Ca^{2+} and H^+ pathways migration simulation was studied by BVSE model.

Keywords: Iron phosphate, Synthesis, X-ray diffraction, Single crystal, Crystal structure, Bond valence analysis, Pathways simulation, Ionic conductor.

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