Short Communication

A New Triphosphate $\text{TlFeHP}_3\text{O}_{10}$: Synthesis, Crystal Structure, Tl^+ and Proton Conduction Pathways

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A new triphosphate $\text{TlFeHP}_3\text{O}_{10}$ was obtained by the hydrothermal method. It crystallizes in the monoclinic space group $C2/c$ with $a=11.994$ (5), $b=8.476$ (2), $c=9.276$ (3), $\beta=111.99$ (3), $V=874.4$ (5) and $Z=4$. The structure was determined by single-crystal X-ray diffraction data collection and provides a clear identification of hydrogen bonds interconnecting the triphosphoric groups in order to build HP_3O_{10} connected by FeO_6 octahedra sharing corners. Thallium cations are located in tunnels. This arrangement was confirmed by CHARDI and BVS models. IR spectrum confirms that most of the vibrational modes are comparable to similar triphosphates and to the calculated frequencies. BVSP and BVSE models were used to simulate conduction pathways migration in the three dimensional framework. The Bond valence analysis revealed that Tl^+ conductivity was one dimensional insured by crystal sites with an activation energy 0.664 eV. However, H^+ conductivity was insured by both crystal sites and interstitials with 0.682 eV migration energy for one dimensional conductivity and 1.293 eV for three dimensional migrations.

Keywords: Triphosphate, Crystal structure, Ionic conductivity, Bond valence analysis, Vibrational study.

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