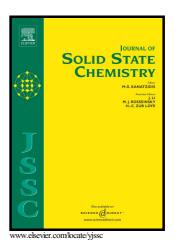
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Two Noncentrosymmetric Polyphosphates Featuring Infinite One-Dimensional $(PO_3)_{\infty}$ Chain, $LiMP_2O_6$ (M = Rb, Cs): Synthesis, Structure and Optical Properties

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Abstract

Two noncentrosymmetric polyphosphates, namely LiCsP₂O₆ and LiRbP₂O₆ have been synthesized from the high temperature solution. The structural analysis suggests that both of them crystallize in orthorhombic space group Fdd2 (No.43), with lattice parameters: a = 18.517(4) Å, b = 19.037(4) Å, c = 13.011(3) Å, and z = 32 for LiRbP₂O₆, while a = 19.009(13) Å, b = 19.402(13) Å, c = 13.180(9) Å, and c = 32 for LiCsP₂O₆. In the structure, the PO₄ polyhedra are connected through corner-sharing to form 1D infinite (PO₃)_∞ chains stretching along the c axis, which are further linked by the LiO₄ polyhedra to construct a 3D framework with two types of tunnels. And the Rb/Cs atoms are filled in or around the periphery of the tunnels to keep the charge equilibrium. The IR spectra verify their structural validity. In addition, other characterizations including the UV-vis-NIR diffuse reflectance spectra, as well as first-principles theoretical studies have been performed on the two compounds.

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