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Two Noncentrosymmetric Polyphosphates Featuring Infinite One-Dimensional $(\text{PO}_3)_\infty$ Chain, LiMP_2O_6 ($M = \text{Rb}, \text{Cs}$): Synthesis, Structure and Optical Properties

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Abstract

Two noncentrosymmetric polyphosphates, namely LiCsP_2O_6 and LiRbP_2O_6 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 LiRbP_2O_6 , while $a = 19.009(13)$ Å, $b = 19.402(13)$ Å, $c = 13.180(9)$ Å, and $Z = 32$ for LiCsP_2O_6 . In the structure, the PO_4 polyhedra are connected through corner-sharing to form 1D infinite $(\text{PO}_3)_\infty$ chains stretching along the c axis, which are further linked by the LiO_4 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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