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Publisher *Taylor & Francis*

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## Phosphorus, Sulfur, and Silicon and the Related Elements

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713618290>

### The Crystal Structure of $\text{LiZn}_2\text{P}_3\text{O}_{10} \cdot 8\text{H}_2\text{O}$

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**To cite this Article** Lutsko, V. , Lyakhov, A. and Prodan, L.(1990) 'The Crystal Structure of  $\text{LiZn}_2\text{P}_3\text{O}_{10} \cdot 8\text{H}_2\text{O}$ ', *Phosphorus, Sulfur, and Silicon and the Related Elements*, 51: 1, 460

**To link to this Article:** DOI: 10.1080/10426509008040984

**URL:** <http://dx.doi.org/10.1080/10426509008040984>

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## THE CRYSTAL STRUCTURE OF $\text{LiZn}_2\text{P}_3\text{O}_{10} \cdot 8\text{H}_2\text{O}$

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The crystal structure of  $\text{LiZn}_2\text{P}_3\text{O}_{10} \cdot 8\text{H}_2\text{O}$  has been determined from three-dimensional X-ray diffraction data collected on Nicolet R3 four-circle diffractometer with CuK-radiation. In the region from  $20^\circ$  up to  $110^\circ$  2016 independent reflections were obtained. Single crystals suitable for X-ray investigation were grown by slow evaporation from the 0.1 mol solution of the composition  $\text{Li}_5\text{P}_3\text{O}_{10}:\text{Zn}(\text{NO}_3)_2=1:1$  at 278 K. The compound belongs to the triclinic space group  $P\bar{1}$  with cell parameters:  $a=10.305(1)$ ,  $b=10.505(1)$ ,  $c=8.671(1)$  Å,  $\alpha=101.79(1)^\circ$ ,  $\beta=113.42(1)^\circ$ ,  $\gamma=94.24(1)^\circ$ ,  $V=830.5$  Å<sup>3</sup>,  $\delta_{\text{calc}}=2.14$  g/cm<sup>3</sup>,  $Z=2$ . The structure was solved by the heavy atom method. The positions of zinc atoms in the unit cell were determined from three-dimensional Patterson function. All other non-hydrogen atoms were located by successive Fourier synthesis. After the last refinement cycles using anisotropic thermal parameters the R value converged to  $R=0.042$  and  $R_w=0.050$ . The bonding of the triphosphate group to the zinc atoms in this structure is bidentate. Zinc atoms have three crystallographically different positions. The tetrahedral coordination two of them is completed by oxygen atoms from triphosphate groups. The third one is octohedrally coordinated by four oxygen atoms from  $\text{P}_3\text{O}_{10}^{5-}$  groups and by two oxygens from water molecules. The tetrahedron of lithium ion is completed by water molecules only. Bond lengths and angles within  $\text{P}_3\text{O}_{10}^{5-}$  group are not fundamentally different from those found in similar chain anions. Zn-O distances range between 1.938 and 2.141 Å while Li-O distances - between 1.939 and 1.969 Å.