

Poster Presentations

[MS18-P10] New compounds in a Cs-Cu-V-P-O system.

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Phosphate-based frameworks incorporating transition and alkaline metals are promising not only as catalysts, sorbents, ion conductors, molecular sieves, but also have the potential to exhibit magnetic and electrochemical properties. Crystals up to 0.2 mm of two new cesium copper vanadyl phosphates, $\text{Cs}_2\text{Cu}(\text{VO}_2)_2(\text{PO}_4)_2$ (I) and $\text{Cs}_2(\text{Cu,Li,V})_3(\text{VO})(\text{P}_2\text{O}_7)_2$ (II) have been obtained by flux crystallization methods in the system Cs-Li-Cu-V-P-O at 700°C. Based on preliminary X-ray diffraction studies it can be assumed that the compound (I) with cell parameters $a = 5.018(6) \text{ \AA}$, $b = 11.589(8) \text{ \AA}$, $c = 9.629(18) \text{ \AA}$, $\beta = 92.76(7)^\circ$, $V = 560.0(7) \text{ \AA}^3$ is isotopic to $\text{Rb}_2\text{Cu}(\text{VO}_2)_2(\text{PO}_4)_2$, studied in [1].

The crystal structure of (II) was determined by single-crystal X-ray diffraction: space group $Pn21a$, $Z = 4$, $a = 13.742(1) \text{ \AA}$, $b = 9.261(1) \text{ \AA}$, $c = 11.551(1) \text{ \AA}$, $V = 1470.0(1) \text{ \AA}^3$. The compound (II) is characterized by a novel structure type. It is based on a mixed three-dimensional framework built from diphosphate $[\text{P}_2\text{O}_7]$ groups, $[(\text{Cu,V,Li})\text{O}_5]$, $[\text{CuO}_5]$ and $[\text{VO}_5]$ tetragonal pyramids sharing vertices. The framework has a system of channels open along the $[001]$ direction. The Cs^+ ions are located in these channels occupying two crystallographically independent positions.

[1] Yakubovich O.V., Steele I.M., Dimitrova O.V. (2008). *Acta Cryst. C.* 64. i62-i65.

Keywords: crystal structure, phosphate, flux method