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New alkali metal diphosphates how materials to preserve the security of the environment: CsNaCu(P2O7), Rb2Cu(P2O7) and CsNaCo(P2O7) synthesis and crystal structure determination

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In this work we describe preliminary results of the synthesis and of a crystal-chemical study of synthetic phosphates with transition metals. Due to the increasing requirements for environmental safety specialists from various industries, we are searching for sustainable forms of immobilization of hazardous waste during storage. We are also developing a component-based waste for new materials. In our continued exploratory synthesis of compounds containing transition-metals, we were able to produce the new diphosphate phases $CsNaCu(P_2O_7)$, $Rb_2Cu(P_2O_7)$ and $CsNaCo(P_2O_7)$.

A crystal chemical study has allowed us to identify new phosphates. Crystals of $CsNaCu(P_2O_7)$ (Phase 1) is orthorhombic, crystallizes in space group *Pmn*2_1, with a = 5.147(8), b = 15.126(2), c = 9.717(2) Å, V = 756.20 Å^3, R_1 = 0.066 and $Rb_2Cu(P_2O_7)$ (Phase 2) is orthorhombic as well, crystallizes in space group *Pmcn*, with a = 5.183(8), b = 10.096(1), c = 15.146(3) Å, V = 793.55 Å^3, R_1 = 0.063, they have been obtained by high-temperature reaction of $RbNO_3$, $CsNO_3$, $Cu(NO_3)_2$, NaOH and $(NH_4)_4P_2O_7$. Synthetic crystals of the phosphate of copper and rubidium were studied in detail by us on the structures of $Rb_2Cu(P_2O_7)$ and $Rb_2Cu_3(P_2O_7)_2$ - new alkali metal copper diphosphates (CHERNYATIEVA et al., 2008). Here we report the synthesis, the structure and the properties of the title compounds and we compare these phases with the previously discovered $K_2CuP_2O_7$ (ELMAADI et al., 1995) and $CsNaMnP_2O_7$ (HUANG et al., 1998). These structures crystallize in other space groups, although their structures are also based on 2-D layers, formed by P_2O_7 groups combined with polyhedra of the transition metals (CHERNYATIEVA et al., 2012).

A crystal chemical study has allowed us to identify even new diphosphates $CsNaCu(P_2O_7)$ (Phase 3). Crystals of $CsNaCoP_2O_7$ is monoclinic, space group $P2_1/n$, with a = 7,424(2), b = 7,648(1), c = 12,931(3)Å, β = 90,71(2)°, V = 734.2(3) Å^3 and R_1 = 0.060. The structure is based framework of Co tetrahedra and P_2O_7 groups. The structure of the $[Co(P_2O_7)]^{2-}$framework in more detail. The phosphate groups and tetrahedra coordinate cobalt ions form topology. This is a unique 4-coordination topology, where Co and P_2O_7 groups in the structure are topologically equivalent.

References

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