New alkali metal diphosphates how materials to preserve the security of the environment: CsNaCu(P2O7), Rb2Cu(P2O7) and CsNaCo(P2O7) syntheses 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(P2O7), Rb2Cu(P2O7) and CsNaCo(P2O7).

A crystal chemical study has allowed us to identify new phosphates. Crystals of CsNaCu(P2O7) (Phase 1) is orthorhombic, crystallizes in space group Pmn21, with a = 5.147(8), b = 15.126(2), c = 9.717(2) Å, V = 756.20 Å3, R1 = 0.066 and Rb2Cu(P2O7) (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 Å3, R1 = 0.063, they have been obtained by high-temperature reaction of RbNO3, CsNO3, Cu(NO3)2, NaOH and (NH4)4P2O7. Synthetic crystals of the phosphate of copper and rubidium were studied in detail by us on the structures of Rb2Cu(P2O7) and Rb2Cu3(P2O7)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 K2CuP2O7 (ELMAADI et al., 1995) and CsNaMnP2O7 (HUANG et al., 1998). These structures crystallize in other space groups, although their structures are also based on 2-D layers, formed by P2O7 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(P2O7) (Phase 3). Crystals of CsNaCoP2O7 is monoclinic, space group P21/n, with a = 7.424(2), b = 7.648(1), c = 12.931(3)Å, β = 90.71(2)°, V = 734.2(3) Å3 and R1 = 0.060. The structure is based framework of Co tetrahedra and P2O7 groups. The structure of the [Co(P2O7)2]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 P2O7 groups in the structure are topologically equivalent.

References


CHERNYATIEVA, A. P, SPIRIDONOV A, D. V., KRIVOVICHEV, S. V. The crystal structures of two new synthetic compounds CsNaCu(P2O7) and Rb2Cu(P2O7), Acta Mineralogica-Petrographica (2012) Vol.7, p.25
