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New alkali metal copper diphosphates: synthesis and crystal structure determination CsNaCu(P2O7), Rb2Cu(P2O7) and Rb2Cu3(P2O7)2

A.P. Chernyatieva, D.V. Spiridonova, and S.V. Krivovichev

Department of Crystallography, Faculty of Geology, St.Petersburg State University, St.Petersburg, Russia (nastya250@yandex.ru)

In this work we describe preliminary results of the synthesis and of a crystal-chemical study of synthetic phosphates with transition metals. We were able to produce the new phosphate phases $CsNaCu(P_2O_7)$, $Rb_2Cu(P_2O_7)$ and $Rb_2Cu_3(P_2O_7)_2$.

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.

A crystal chemical study has allowed us to identify even new diphosphates, like $Rb_2Cu_3(P_2O_7)_2$ (Phase 3). It is orthorhombic and crystallizes in space group $P2_12_12_1$, with a = 9.941(1), b = 13.475(1), c = 18.635(1)Å, V = 2496.4(2) Å^3, R_1 = 0.075. The structure consists of an anionic framework $[Cu_3(P_2O_7)_2]^-$, which is found in the channels, located in the cavities of the cations Rb^+, which occupy three independent positions (Rb1, Rb2, Rb3). The structure contains six crystallographically independent copper atoms, which connect the diphosphate complexes in the framework, via Cu-O.

References

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