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# New f-element phosphates with langbeinite-type structure

Crystal chemical principle allows to create new compounds with expected structure and properties. In this work it was used for "constructing"new f-element phosphates with langbeinite type structure (Lb). Earlier we used this approach for calculation of formula cation compositions of tetrahedral-octahedral frameworks for NZP and Lb forms [1], then some new phosphates with Lb structure were prepared [2-4]. These are phosphates: K2RZr(PO4)3, R=Pr-Lu,Y; K2R3/2Ta1/2Zr(PO4)3, R=Gd-Yb,Y; A2RZr(PO4)3, A=Rb,Cs; R=Pr,Er; KBaR2(PO4)3, R=Yb,Er; CsBaR2(PO4)3, R=Dy-Yb; ABaFe2-xPrx(PO4)3, A=K,Cs, x=0,25; 0,5; 0,75.

As a development of this research we have calculated the formula phosphate compositions with expected Lb-type structure with 3- and 4-valent elements in the interframework sites: [A3/2R1/2]3+; [A5/3M1/3]3+; [AR]4+; [A4/3M2/3]4+, A,R,M −1-,3-,4-valent cations, also f-elements. We were going to prepare the phosphates: A3/2Ln1/2MgZr(PO4)3, A3/2Ln1/2Fe2(PO4)3 and ALnMg3/2Zr1/2(PO4)3, where A = K, Rb, Cs; Ln = Pr, Sm, Yb. Synthesis was carried out by sol-gel technology. The IR, X-Ray and DSC analysis have been used for samples characterization.

We have established the optimal conditions: pH = 7-9; T=600 and 800˚C during 24 h on every stages, quick addition of H3PO4 solution; Ultrasonic activation wasn't effective.

The phosphates A3/2Ln1/2MgZr(PO4)3 and A3/2Ln1/2Fe2(PO4)3 higher presented with cubic structure, sp. gr. P213 were formed. An attempts to prepare phosphates with bigger concentration of Ln-cations in the interframework positions such as ALn or A1.2Ln0.8 wern't successful. The additional X-Ray reflections of the monazite type phases presented on XRD patterns. Monazite phase as an admixture also presented in all phosphate samples prepared.

The temperature limits of existence of Lb type phases were established: from 750 - 800 up to 900 - 1150 ℃. The thermal decomposition products were identified as phosphates with NZP- or monazite-type structures and as phosphate Cs7Fe7(PO4)8O2 in the case of iron-containing compounds.

The lanthanide ions in LnOn polyhedra in the structure of new phosphates are characterized by ninefold coordination in cavities. In known phosphates with such structure with Ln-cations located in framework sites the coordination is n = 6 [2, 3].

Crystal chemical principle allows to predict new phosphate compositions with expected Lb-type structure containing lanthanide cations in sites of both types simultaneously. This may be realized as the subject of future investigations.

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