Phase diagram of the BaF_2 - YF_3 system

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The BaY_2F_8 compound has recently been the subject of numerous studies, especially regarding the spectroscopy of neodymium-doped crystals. Very few studies, however, deal with the phase relations of its constituent compounds, the BaF_2 and the YF_3; the present work therefore focuses on the investigation of the phase relations of the BaF_2 - YF_3 system, with the particular intent of better understanding the growth process of BaY_2F_8 crystals. Crystallized samples of diverse compositions have been prepared and were subjected to thermal analysis techniques (differential thermal analysis, differential scanning calorimetry and thermogravimetry). Discrepancies between the results and the phase diagrams found in the literature[1,2] have been observed and are currently under investigation. The samples have also been subjected to analysis via X-ray powder diffraction and quantitative calculation of phase concentrations using the Rietveld method; lattice parameters of the BaY_2F_8 monoclinic structure were also calculated. (This work was supported by CNPq and CAPES)

[1] N.L. Tkachenko, M. Svantner, B.P. Sobolev, Inorganic Materials (USSR) (Engl. Tranl.) 13 (5), (1977) 693.

[2] Tkachenko, N.L.; Garashin S.L.; Phase Equilibria in BaF2-(Y,Ln)F3 Systems; Journal of the Solid State Chemistry (USSR) (Tradução para o Inglês), 8 (3), (1973) 213-218.