Structural and thermal investigation in RbB(SO₄)₂.4H₂O - RBS (B=Nd, Sm, Eu) single crystal.

E. Dórico^a, K. M. Novack^b, G. J. Perpétuo^c and C. J. Franco^c.

^aDepartamento de Física, Universidade Federal de Santa Catarina, Florianópolis, Brasil. ^bDepartamento de Química, Universidade Federal de Ouro Preto, Ouro Preto, Brasil. ^cDepartamento de Física, Universidade Federal de Ouro Preto, Ouro Preto, Brasil.

The isostructural materials series $AB(SO_4)_2.4H_2O - ABS$ (A=Rb, NH₄, B=Nd, Sm, Eu, La, Ce, Pr, Gd, Tb, Dy) were promising to investigate the phase transition behavior and the effect of the replacement of monovalent and trivalent cations on the crystal structure and, consequently, compare the phase transition behaviors of the ammonium and rubidium compounds[1, 2].

Good prismatic crystals of $RbB(SO_4)_2.4H_2O - RBS$ (B=Nd, Sm, Eu) were grown by isothermal evaporation at 35^oC from aqueous solution of B₂(SO₄)₃.8H₂O (B=Nd, Sm, Eu) and Rb₂SO₄, mixed in the molar ratio 1:3.

The crystal structure of RbNd(SO4)2.4H2O – RNdS was investigate at 25° C, -48° C, -96° C and -153° C and in RbEu(SO4)2.4H2O – REuS at 25° C and -153° C.

The unit cell in RNdS and REuS at 25° C is monoclinic with P2₁/c space group and at -153° C is triclinic with P1 space group with unit cell triplicate in RNdS and duplicate in REuS.

At room temperature the structure of this crystal can be envisioned as consisting of one polyhedron of lanthanide ions, two crystallographically independent sulfate tetrahedra and one rubidium polyhedron.

Dehydration investigated by TG/DTA and DSC in RBS (B=Nd, Sm, Eu) shows that these crystals loss their four water moles between 100° C and 280° C according of the general rule RbB(SO₄)₂.4H₂O \rightarrow RbB(SO₄)₂+4H₂O[3].

At temperatures above 380^oC two exothermal peaks were detected suggesting the formation of ordered structures as suggested by x-ray powder diffraction measurements. FTIR and UV results are also presented and discussed.

On the base of our data and the literature a phase diagram is proposed for the description of rubidium lanthanide crystal family[4].

References:

[1] Sastry, J., Robinson, P. D., Malhotra, V. M., Phys. Rev. B, 43, p. 13215-13227 (1991).

[2] Misra, S. K., Isber, S., and Li, L., J. Phys: Condens. Matter, 10, p. 10667-10677 (1998).

[3] Dórico, E. *Análise estrutural de compostos de lantanídeos tetrahidratados*. Dissertação (Mestrado em Rede Temática Em Engenharia de Materiais Redemat) – UFOP, Ouro Preto, 2004.

[4] Dórico, E., Novack, K.M., Perpétuo, G. J., and Franco, C. J., Manuscript to be submeted.

Acknowledgment: FAPEMIG; CNPq; UFOP.