

lized as excitation source. The absorption spectra of the solution analyzed were recorded using a spectrophotometer. The x-ray powder diffraction pattern of crystals shows that below 60 % of Nickel sulfate in the solutions in which the crystals grow the crystals crystallizes in triclinic structure but above 60 % of Nickel sulfate the crystals crystallizes in orthorhombic structure. In order to complement the result obtained by the X-ray analysis, we have performed Raman measurements at room temperature over the spectral range from 10 nm to 1400 nm confirming that below 60 % of Nickel sulfate in the solutions in which the crystals grow the crystals crystallizes in triclinic structure but above 60 % of Nickel sulfate the crystals crystallizes in tetragonal structure. Optical transmission spectra reveal that crystals grow with orthorhombic structure has an absorption band at 350 - 450 nm.

[12/05/10 - P038]

EXAFS and XANES of Ca₂MnReO₆ under pressure up to 1.2 GPa, DANILO O. DE SOUZA,

M. T. D. ORLANDO, *Universidade Federal do Espírito Santo*, H. P. S. CORRÊA, *UFMS*, J. L. ROSSI, L. G. MARTINEZ, *IPEN*, F. C. L. MELO, *CTA* ■

Double perovskite materials have been attracted renewed interest in early years because the of large low-field room-temperature magnetoresistance in these compounds (mainly in half-metallic Sr₂FeMoO₆, described by Kobayashi in 1998) stimulated interest in the study of the properties of ordered double perovskites, in the context of their potential application in the field of spin electronics. This type of compound exhibits magnetic and electronic properties related to the strong interplay between structure, charge and spin ordering, which is the subject of nano-spintronic studies. This work was proposed by taking into account a scenario which the magnetic and electronics properties of the Ca₂MnReO₆ double perovskite present a strong correlation with structural order. The main goal was to investigate the synthesis and crystal structure of the monophasic compound Ca₂MnReO₆. EXAFS measurements at ambient pressure were performed in order to determine the ReO₆ and MnO₆ octahedral coordination in the Ca₂MnReO₆ double perovskite. The valence of Mn and Re was determined taken into account the MnO, MnO₂, ReO₂ and ReO₃ calibrators. EXAFS pattern behavior of ReO₆ and MnO₆ octahedral was also investigated under hydrostatic pressure up to 1.2 GPa. A CuBe pressure cell with B4C anvils was used to applied pressure in situ. Our conclusions are that the both octahedral present a tilt under pressure without change its Re-O and Mn-O coordination distances.

[12/05/10 - P039]

Structural and thermal investigation of RbB(SO₄)₂·4H₂O B=Nd, Sm, Eu crystal,

ERILDO DORICO, , CARLOS JOEL FRANCO, GENIVALDO JÚLIO PERPÉTUO, *UFOP* ■ Good prismatic crystals of RbB(SO₄)₂·4H₂O - RBS (B=Nd, Sm, Eu) were grown by isothermal evaporation at 35 C from aqueous solution. This crystal family were investigated by Electron Paramagnetic Resonance, X-ray diffractometry, specific heat in order to obtain information of the crystal structure and their properties. In this work

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 the general rule RbB(SO₄)₂·4H₂O converted in RbB(SO₄)₂ and 4H₂O. At temperatures above 380 C two exothermal peaks were detected suggesting the formation of ordered structures as suggested by x-ray powder diffraction measurements. On the base of our data and the literature a phase diagram is proposed for the rubidium lanthanide crystal family.

Acknowledgment: FAPEMIG, CNPq, UFOP.

[12/05/10 - P040]

Growth and characterization of l-histidine-Cl crystal., CARLOS JOEL FRANCO, FABRICIO MENDES

SOUZA, GENIVALDO JÚLIO PERPÉTUO, RODRIGO FERNANDO BIANCHI, *UFOP* ■ The discovery of the non-linear optical (NLO) in L-Arg.H₃PO₄.H₂O (LAP) (where L-Arg is L-arginine) has a major role in attracting attention to the crystalline salts of amino acids. The L-histidine (L-His) has the chemical formula (N₂C₃H₃CH₂CH(NH₂)COOH) similar to L-Arg. New crystals that exhibit ONL can be obtained from salts of the amino acid L-histidine and HCl acid. The reaction of L-His with several other acids (HBr, HF and H₂C₂O₄) can also produce materials that have ONL effects to be studied. Good single crystals of L-His + HCl + H₂O were grown and characterized by TG-DTA and X-ray . These types of crystals are great generators of second harmonic. Crystal Chlorine L-His with a volume of 0.5 x0, 5x1cm³ are being grown in our laboratory by the method of solution in a beaker with about 50ml of solution. Solution of L-his + HCl (aq) was prepared with 5.0000 g of L-histidine and approximately 2.30 ml of HCl with a density of 1.19 g / mL. This solution was saturated in the heater-shaker and placed in an oven for evaporation. This procedure was performed on several occasions to obtain crystals with possible differences in their crystal structures. In order to understand the stability of the crystal of chlorine L-histidine with temperature we performed measures thermogravimetry TG / DTA and DSC from room temperature and to 500 C. Through analysis of the chart may be concluding that after heating the samples Chlorine L-His may be the loss of small molecules such as H₂O, NH₃ and CO₂. Our results show a rich thermal process between 250 and 350 C. Were also carried out measures to verify the generation of second harmonic. Through measures x-ray and Raman characterize the structure of crystals Chlorine L-His obtained. The results will be discussed and presented in detail.

Acknowledgment: FAPEMIG, CNPq, UFOP.