Low Temperature Stability of Fluoride Pyrochlores investigated by Neutron Powder Diffraction and Raman Spectroscopy

Eder Nascimento Silva[a], Alejandro Ayala[a], Ilde Guedes[a], Josué Mendes Filho[a], Chun Long[b], Jean Gesland[c], *[a]Depto. de Física, Universidade Federal do Ceará, Fortaleza, Brazil. [b]Argonne National Laboratory, Argonne, Illinois, USA. [c] Université du Maine Cristallogenese, Le Mans Cedex, France.* E-mail: eder@fisica.ufc.br

Compounds that are isoestructural to the mineral pyrochlore $((NaCa)_2(NbTa)_2O_6(F/OH)$ form a populous family with more than 150 members. All of these compounds have a regular or distorted pyrochlore structure, which has the form $A_2B_2X_6X'$ (where X and X' = O, F, S, OH), a face centered cubic lattice belonging to the *Fd-3m* space group and eight formulas per unit cell. Two families of fluoride compounds are known to crystallize in the pyrochlore structure: $A(M^{2+}_{1/2}M'^{3+}_{1/2})_2F_6$ (the A_2X' sublattice is replaced by larger monovalent cations, such as Cs^+ and Rb^+) and $(A^{1+}_{1/2}A'^{2+}_{1/2})_2B^{2+}_2F_7$ or, in a more compact form, $AM^{2+}M'^{3+}F_6$ and $A^{1+}A'^{2+}B^{2+}_2F_7$, respectively. Recent measurements of polarized Raman scattering and infrared reflectance spectroscopy suggested a disorder induced local symmetry lowering, even though x-ray diffraction results confirmed an average pyrochlore structure. Thus, the aim if this work is to investigated the low temperature stability of the fluoride pyrochlore structure of compounds belonging to both families by neutron powder diffraction and Raman spectroscopy.

Acknowledgements: The authors thank to IPNS/ANL (Project 4132/04) and to Dra. Simine Short for the neutron diffraction measurements. The authors also thank to CNPq and CAPES for the financial support.

Keywords: pyrochlore, symmetry breaking, Raman scattering