Structural and optical properties of rare earth doped BaY_2F_8

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Mixed metal fluorides, when doped with rare-earth ions (RE), are promissing materials for solid-state optical devices. BaY_2F_8 is a suitable host for RE incorporation and already have applications as a laser in the IR region. In the present work, we report the optical properties of the rare-earth doped BaY_2F_8 and its potential use as a scintillator in radiation detection. The synthesis of RE-doped BaY_2F_8 was performed in a platinum reactor from stoichiometric mixture of BaY_2F_8. Tb, Nd and Tm are added in concentrations from 0.5 to 3molX-ray powder diffraction was performed in the synthesized powders and in the crystals and quantitative phase analysis were done using the Rietveld method. Additionally to the determination of the phase concentrations, lattice parameters, fractional atomic coordinates, site-occupancies and anisotropic thermal parameters were refined in the analyses. Absorption, emission and excitation spectra of the doped samples were measured at room temperature. The identification of the transitions was done comparing the absorption, excitation and emission peaks with the results obtained form computer modelling. The modelling strategy includes the relaxation of the surrounding ions and then calculating the crystal field parameters (B_q^k)from the relaxed structure. The set of non-zero B_q^k determines the local symmetry of the RE ion and were input in the calculation of the 4f energy levels splitting. The scintilator properties of the pure and doped samples were checked measuring the radioluminescence of the sample when excited with different types of radiation, (gamma, beta, X-rays, and ion beams), revealing that these materials are promising radiation detectors.(This work was partially funded by MCT/PADCTII/CNPq, FINEP and CAPES)