

# Luminescent Properties of Hydrothermally Synthesized Pr<sup>3+</sup>Doped Barium Lutetium Fluoride Nanocomposite Material

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In recent years, ternary fluoride compounds have gained significant attention for their potential applications as scintillators offering ultrafast response times crucial for medical imaging in time-of-flight positron emission tomography, as well as for high-energy physics calorimetry and X-ray photodynamic therapy<sup>1,2</sup>. Among these, ternary fluoride compounds doped with Pr<sup>3+</sup> ions have particularly sparked interest due to their ability to exhibit either strong 4f<sup>1</sup>5d<sup>1</sup>→4f<sup>2</sup> emissions in the UV region or a cascade of the 4f<sup>2</sup>→4f<sup>2</sup> emissions in the visible region, depending on the crystal field strength influencing the position of the 4f<sup>1</sup>5d<sup>1</sup> state in the electronic band structure of the compound<sup>3</sup>. To explore the potential of such compounds, in this study, we focused on synthesizing Pr<sup>3+</sup> ion doped barium lutetium fluoride composite material via a hydrothermal process. X-ray diffraction analysis revealed that the composite material consisted of two phases: an orthorhombic phase (BaLu<sub>2</sub>F<sub>8</sub>) comprising 89% of the material and a cubic phase (BaLuF<sub>5</sub>) comprising 11%. Scanning transmission electron microscopy confirmed the presence of these two distinct phases, with BaLuF<sub>5</sub> exhibiting a spherical morphology and BaLu<sub>2</sub>F<sub>8</sub> displaying elongated plate like morphology.

Time-integrated (TI) luminescence spectroscopy conducted under vacuum ultraviolet (VUV) photon excitation at the FinEstBeAMS beamline revealed interesting findings. In the orthorhombic phase of the nanocomposite, the Pr<sup>3+</sup> 4f<sup>1</sup>5d<sup>1</sup> bands were found to be positioned below the 4f<sup>2</sup> <sup>1</sup>S<sub>0</sub> energy level, whereas in the cubic phase, it remained above the same energy level. Consequently, upon the high-energy (45 eV) and Pr<sup>3+</sup> 4f<sup>1</sup>5d<sup>1</sup> excitation (6.75 eV), the nanocomposite demonstrated broad UV emission bands from the orthorhombic phase, attributed to the 4f<sup>1</sup>5d<sup>1</sup>→<sup>3</sup>H<sub>4,5,6</sub> transitions (4.4 to 5.8 eV), as well as narrow lines in the UV-visible region from the cubic phase, arising due to a two-step photon cascade emission process involving the <sup>1</sup>S<sub>0</sub>→<sup>1</sup>I<sub>6</sub> (3.04 eV) and <sup>3</sup>P<sub>0</sub>→<sup>3</sup>H<sub>4,5,6</sub> (2.68 eV–1.80 eV) transitions. Additionally, decay kinetics studies indicated a fast decay of the emissions related to 4f<sup>1</sup>5d<sup>1</sup>→<sup>3</sup>H<sub>4,5,6</sub> transitions from the orthorhombic phase (τ~11 ns), contrasted with a relatively slow emissions from <sup>1</sup>S<sub>0</sub>→<sup>1</sup>I<sub>6</sub> transitions from the cubic phase (τ~102 ns). These findings underscore the potential of this composite material to generate both UV and visible emissions, highlighting its potential for applications in various medical applications. The relaxation processes leading to various emissions in the mixed phase composite will be discussed on the basis of experimental data analysis.

## References

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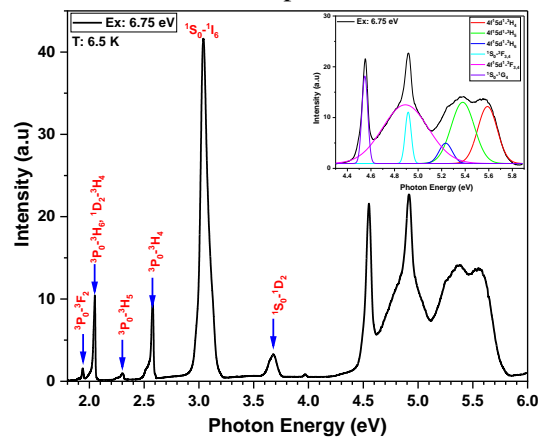


Figure 1: TI photoluminescence spectra of Pr<sup>3+</sup> doped barium lutetium fluoride nanocomposite under excitation to the Pr<sup>3+</sup> 4f<sup>1</sup>5d<sup>1</sup> state (6.75 eV) at 6.5 K.