





Belo Horizonte, September 12 - 15<sup>th</sup> 2024

## GdF<sub>3</sub> structure distortion effect with Eu<sup>3+</sup> doping.

## Gustavo C. Portes<sup>1</sup>, Lucca Blois<sup>1</sup>, Hermi F. de Brito<sup>1</sup> and Lucas C. V. Rodrigues<sup>1</sup>

<sup>1</sup>Department of Fundamental Chemistry, Institute of Chemistry, University of São Paulo, São Paulo, Brazil

E-mail:qustavo.portes@usp.br

Thematic Area: Rare Earths

**Keywords**: Lanthanides, Structure distortion, Luminescence.

Trivalent Rare earth ions (RE<sup>3+</sup>) exhibit luminescence related to 4f-4f transitions, which are considered forbidden by Laporte's rule. However, these transitions are observed due to relaxations of this rule. Since the 4f orbital is shielded by the 5s and 5p orbitals, its interaction with the ligand can be considered as mainly electrostatic.

Trivalent europium has a sharp emission spectrum that presents a fine structure dependent on the interaction between the metal ion and the crystal field. These emissions are well-known, with its most intense emission being the  ${}^5D_0 \rightarrow {}^7F_2$  transition in the 611 nm region, giving the Eu³+ luminescence a reddish color. This emission being hypersensitive to the symmetry of the matrix, with intensity loss depending on the ion's position in the crystalline structure, makes it possible to use the Eu³+ as a structural probe when used as a dopant, in order to increase the understanding of the chemical environment around the metal ion.

The GdF<sub>3</sub> matrix can be synthesized in hexagonal and orthorhombic forms, both of which have a center of inversion. When doped with Eu<sup>3+</sup>, the most intense emission is the  ${}^5D_0 \rightarrow {}^7F_1$ , which appears in the 593 nm region. The  ${}^5D_0 \rightarrow {}^7F_2$  emission is more sensitive to the inversion center and, in this case, occurs with lower intensity due to vibronic interactions. However, when the europium doping is increased, a change in the emission color is noticeable.

In this work, we studied this change through X-ray diffraction and fluorescence spectroscopy analyses to determine if there is a distortion in the  $GdF_3$  crystal lattice due to the high percentage of dopant, thereby reducing the effects of the inversion center and increasing the 611 nm emission intensity of  $Eu^{3+}$ .

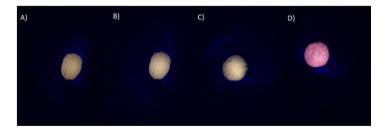


Figure: Luminescence of GdF<sub>3</sub> with A)0,1%, B)0,5%, C)1,0% and D)5,0% Eu<sup>3+</sup> doping.

Acknowledgments: FAPESP(2021/08111-2), CAPES (process: 88887.825181/2023-00) References

- [1] G. Vicentini et al., Coordination Chemistry Reviews, 196, 353-382 (2000).
- [2] X. Zhang et al., Journal of Alloys and Compounds, 509, 2076-2080 (2011).