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Luminescent studies of europium (III) fluorobenzoic acid derivatives: Correlating the calculated electronic energies and the experimental luminescent efficiencies through computational studies

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Europium (III)-based luminescent complexes promise extensive potential applications in immunoassay technology, high throughput drug screening, organic light emitting diodes (OLEDs), and biomedical imaging. Europium-ligand complexes present unique properties such as monochromatic emission at 614 nm, long luminescent lifetimes enabling time-resolved measurements, minimal photobleaching, and large Stokes shifts. Ligand design for enhancing the quantum efficiency of europium complexes is currently active. For this reason, it is important to understand the electronic mechanisms that allow europium-metal complexes to fluoresce. Here, we report the structural and spectroscopic properties of a series of europium (III) complexes containing fluorobenzoic acid derivatives using density functional theory calculations. Calculations were carried out using the B3LYP method and 6-31G* and 6-311+G** basis sets. Upon increasing the ligand fluorination, the absorption maximum wavelength shows a blue shift. Excited state energy gaps of the complexes were found to be sensitive to the identity and the position of the ligand substituents. A nitro substitution results in a decrement of the vertical excited states, significantly reducing the luminescent quantum yield. The inter-system crossing energy gap is strongly regulated by the position of the ligand substituent. It is significantly reduced by having substituents closer to the metal coordination site. The optimum energy gaps resulting in enhanced luminescent quantum yields were identified. The correlation among the calculated experimental luminescent quantum yields and the calculated electronic energy levels will be discussed to provide insight into designing highly luminescent europium complexes.

Keywords: Europium complexes, excited states, density functional theory, computational chemistry, quantum yield

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