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Europium(III) complex with powerful antenna ligands: interligand interaction

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Abstract

The luminescent properties of europium(III) trifluoroacetate [Eu(TFA)3bipy·3H2O]·bipy (**I**), where TFA – trifluoroacetate anion and bipy – 2,2′bipyridyl were investigated. Despite the presence of two efficient antenna ligands in complex (bipy1 in europium coordination sphere and bipy2 in the outer-sphere) the complex displays weak luminescence. By employing density functional theory-based methods, the luminescence, electron structure, interligand interactions and the processes of energy transfer in **I** were investigated. The nature of the chemical bond in **I** was studied by the natural bond orbital analysis. The mechanism of luminescence weakening in the complex was ascertained: competitive energy transfer from coordinated bipy1 ligand on to outer-sphere bipy2 molecule results in appreciable weakening of the antenna effect.

Keywords: Luminescence, antenna effect, quantum chemistry, DFT, interligand interaction

1. Introduction

Working out of intense luminescent and photostable functional materials based on the rare-earth complex compounds for optoelectronics (LEDs and OLEDs), analytical chemistry, agriculture, and medicine is a topical task [1-4].

Study of the photophysical properties of lanthanide coordination compounds is necessary for targeted synthesis of new luminescent rare-earth compounds. Intense luminescent, triboluminescent, sensor and photochemical properties of rare-earth complexes let to use them as dopants for functional optic materials (light-