

Accepted Manuscript

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

T.B. Emelina, I.V. Kalinovskaya, A.G. Mirochnik



PII: S1386-1425(18)30857-6
DOI: doi:[10.1016/j.saa.2018.09.012](https://doi.org/10.1016/j.saa.2018.09.012)
Reference: SAA 16453

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 7 May 2018
Revised date: 6 August 2018
Accepted date: 8 September 2018

Please cite this article as: T.B. Emelina, I.V. Kalinovskaya, A.G. Mirochnik , Europium(III) complex with powerful antenna ligands: Interligand interaction. Saa (2018), doi:[10.1016/j.saa.2018.09.012](https://doi.org/10.1016/j.saa.2018.09.012)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

УДК 548.73:548.75:546.65

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

T.B.Emelina*, I.V.Kalinovskaya, A.G.Mirochnik

Institute of Chemistry, Far East Branch of the Russian Academy of Sciences,

Vladivostok, 690022 Russia

maks-im2@mail.ru

Abstract

The luminescent properties of europium(III) trifluoroacetate $[\text{Eu}(\text{TFA})_3\text{bipy}\cdot 3\text{H}_2\text{O}]\cdot\text{bipy}$ (**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-

Download English Version:

<https://daneshyari.com/en/article/10147317>

Download Persian Version:

<https://daneshyari.com/article/10147317>

[Daneshyari.com](https://daneshyari.com)