

---

**THE INFLUENCE OF THE NATURE OF  
SUBSTITUENTS ON LUMINESCENCE  
PROPERTIES OF MESOGENIC EUROPIUM(III)  
COMPLEXES**

---

<sup>1</sup>Physical and Colloid Chemistry Department, Kazan National Research Technological University, Karl Marx Str., 68, Kazan, Russia

---

*kseuyua@mail.ru*

---

Lanthanide-containing materials exhibit remarkable magnetic and optical properties due to the 4*f*, 5*p*, and 5*d* electronic structure of Ln(III) ion, and are widely used in various fields of applications. The numerous studies are concentrated on europium(III) (Eu) coordination compounds with organic ligands (mostly  $\beta$ -diketons) which can be used as the most efficient red emitters for optoelectronic devices, organic light emitting diodes, solar batteries, and luminescence biological probes [1]. Organic ligands in these molecules provide the transfer of the excitation energy onto the emissive Ln(III) ion. Computer simulations can help one to find the ligands that provide the most efficient energy transfer to the Ln(III) ion and simplify the design of highly efficient luminescence materials. In this study, the influence of the substituents in the structure of  $\beta$ -diketons on luminescent properties of some mesogenic Eu(III) complexes was investigated. Quantum-chemical methods were applied for the simulation of equilibrium geometries, excited states and absorption spectra of Eu(III) complexes with different ligand environment.

The optimization of molecular geometry and IR spectra calculations were made using the density functional theory and the exchange-correlation functional PBE. NMR simulations were carried out by GIAO method. The energies of the lowest singlet and triplet excited states were calculated by TDDFT method (PBE, B3LYP) in program Firefly 8. For Eu(III) ion the scalar relativistic 4*f*-in-core pseudopotential ECP52MWB with the associated valence basis set was used and 6-31G(d,p) basis set - for other atoms. The calculations of UV absorption spectra were made using Sparkle method in ORCA 3.0.3 program.

Influence of the nature of substituents on optical properties of the complexes and the effectiveness of their use in optoelectronics was revealed. The calculated UV, IR, NMR spectra and the excited states were confirmed experimentally. Correlations between the positions of the excited levels and the values of absolute quantum yield were established, the main intramolecular energy transfer channels were determined. It was found that during the photoexcitation the greatest contribution comes from  $\beta$ -diketones whose geometry considerably changes in comparison with other ligands.

The calculations were performed using the facilities of the Joint Supercomputer Center of Russian Academy of Sciences and the Supercomputing Center of Lomonosov, Moscow State University [2].

---

1. Romanova K.A. et al. *Journal of Physical Chemistry A*, 2014, **118**: 11244-11252.

2. Voevodin V.V. et al. *Open Systems Journal*, 2012, **7**: 36-39.

---

*This work was supported by the grant of the President of the Russian Federation for the state support of the young Russian scientists - candidates of sciences (No MK-7320.2016.3).*

---