Luminescent properties of europium-EDTA complexes with 2-acyl-1,3-indandionate ligands

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This work reports the synthesis and investigation of the structural and luminescent properties of aqueous-soluble lanthanide ion complexes, containing the ethylenediaminetetraacetic acid (EDTA) ligands and the classes of aliphatic b-diketonate and 2-acyl-1,3-indandionates. The spectroscopic properties of complexes with the formula $[Ln(EDTA)L]^-$ were intensively investigated using absorption and luminescence spectroscopy data recorded in aqueous solution. Theoretical calculations using density functional theory (DFT) at the ωB97XD3/MWB52/Def2-SVP level of theory, employing the Gaussian Def2-SVP basis set for the H, C, O, F, and S atoms, and the Stuttgart-Dresden “large-core” MWB52 effective potential together with its valence basis set [7s6p5d]/[5s4p3d]-GTO for the Eu^{3+} ion, were performed in order to obtain the ground-state geometries of the complex molecules. In addition, the spectroscopic properties of the systems were also investigated based on time-dependent density functional theory (TD-DFT) calculations at this same level of theory. Furthermore, the first coordination sphere of lanthanide ions was investigated theoretically, using recent theoretical methodologies implemented in the JOYSPECTRA platform. The experimental results of the average excited state lifetimes (t), intensity parameters W_2 and W_4, radiative (A_{rad}) and non-radiative (A_{nrad}) decay rates, and intrinsic quantum yield of the Eu^{3+} ion (Q^{Eu}) suggested changes in the chemical environment with the coordination of the diketonate ligands, resulting in higher luminescence intensities. The theoretical data also demonstrated that the most efficient mechanism for energy transfer involves the excited triplet state located in the diketonate ligands.

Acknowledgements
The authors acknowledge CNPq, CAPES, FINEP and FAPESP for financial support

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