Production of new luminescent rare earths coordination compounds

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Research area on lanthanide-based luminescent coordination compounds is very promising, especially due to their application in biomedics and optics technologies. These applications depend directly on the electronic structure of rare earths ions, but also on the coordination compounds molecular structures. Lanthanide-based coordination compounds usually show narrow emission bands, intense luminescence, and long excited state lifetimes, therefore, they have attracted considerable interest as luminescent probes. Thiabendazole (TBZ) is an antimicrobial drug from benzimidazole derivatives and its structure presents an efficient coordination with transition metals [1]. Trisodium 4,4'-(3-(4-(4-sulfonatophenyl)pyridin-2-yl)-1,2,4-triazine-5,6-diyl)dibenzenesulfonate (SPT) is a bulky aromatic molecule where a sophisticated multinuclear coordination compounds structurally can be synthesized. The aims of this work were to synthesize new luminescent compounds and investigate their spectroscopic properties. The compounds were synthesized in an alcoholic solution using a 2:1 ligand:metal molar ratio. TBZTb and SPTEu were prepared using pentahydrate nitrates of terbium (Tb) and europium (Eu), respectively. These compounds were characterized by infrared (IR) and photoluminescence (PL) spectroscopies, and thermogravimetric analysis (TGA). Free ligands were used as reference standards. TBZTb IR spectra showed shifted bands from 1621 cm^{-1} to 1627 cm^{-1} and 1579 cm^{-1} to 1594 cm^{-1} (νC=N and νC=C, respectively) from imidazole and thiazole rings. The band at 740 cm^{-1} assigned to νC-S suffered any change, thus suggesting Tb coordination through nitrogen sites. In addition, νN-H appeared as a large band at 2800 – 2600 cm^{-1} due to hydrogen bonding on the free TBZ spectrum. However, this interaction was probably broken during the coordination process, since this stretching appeared as a single band at 3500 cm^{-1} on the IR complex spectrum. SPTEu IR spectra showed shifting at 1620-1520 cm^{-1} assigned to pyridine and 1,2,4-triazine ring, and at 1370-1120 cm^{-1} (intense band) assigned to sulfonate group ($R\text{-}SO^{3-}$). Those results suggested a possible Eu^{3+} coordination mode to SPT ligand through nitrogen and oxygen sites. PL results showed characteristics emission spectra for SPTEu and TBZTb with maximum emission bands, respectively, at 614 nm (λ_{ex} = 360 nm), due to $^5D_o \rightarrow {}^7F_2$ (Eu, red – Fig. 1) electronic transition, and 542 nm (λ_{ex} = 340 nm), due to $^5D_4 \rightarrow {}^7F_5$ (Tb, green – Fig. 1) electronic transition. Quantum efficiency of 20% was obtained for SPTEu and quantum yield of 35% was calculated for TBZTb. From TGA results, it was possible to estimate molecular formula for both complexes resulting in $[Eu(SPT)]\cdot 5H_2O$ and $[TbTBZ_2(NO_3)_3]\cdot 2H_2O$, for SPTEu and TBZTb, respectively. Materials thermal stability was also investigated. [1] Mothilal, K. K.; Karunakaran, C.; Rajendran, A.; Murugesan, R.; *J. Inor. Biochem*. **2004**, *98*, 322. [2] Ailing Wang, A.; Wei, X.; Zhang, H.; Yue, B.; Qu, Y.; Kang, J.; Wang, Z.; Chu, H.; Zhao, Y.; *Dalton Trans*. **2014**, *43*, 2620. UFES, NCQP, FAPES and CAPES.

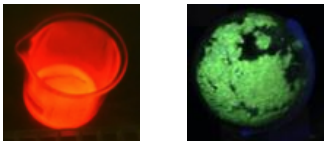

Fig. 1. SPTEu red emission; TBZTb green emission