

P43: The Influence of the *Odd-Even Effect* of Aliphatic Dicarboxylate Ligands on the Photoluminescent Properties of Europium Complexes

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Eleven $[\text{Eu}_2(\text{L})_3(\text{H}_2\text{O})_x] \cdot y(\text{H}_2\text{O})$ complexes with aliphatic dicarboxylate ligands (L: OXA, MAL, SUC, GLU, ADP, PIM, SUB, AZL, SEB, UND, and DOD, where $x=2-6$ and $y=0-4$) were synthesized and characterized by elemental and thermal analysis, FTIR spectroscopy and powder X-ray diffraction. The obtained data confirms the ligand to metal ratio, the hydration degree, the coordination mode and that the complexes are crystalline. The *oddeven effect* was observed for the final dehydration temperature of the Eu^{3+} complexes (Fig. 1). Moreover, the effect was also observed in the experimental and theoretical photoluminescent properties such as the intensity parameters, Ω_2 and Ω_4 (Fig. 2) and the emission intrinsic quantum yield, Q_{Ln}^{Ln} (Fig. 3) of the Eu^{3+} complexes. The *oddeven effect* on the Ω_2 and Ω_4 values could be explained by using an extension of the dynamic coupling mechanism, herein named the ghost-atom (GA) model, in which the long-range polarizabilities (α^*) were determined by simulating the presence of a ghost atom in the middle of each ligand carbon chain and the localized molecular orbital approach. The GA approach is an extension of the Bond Overlap Model (BOM) [1].

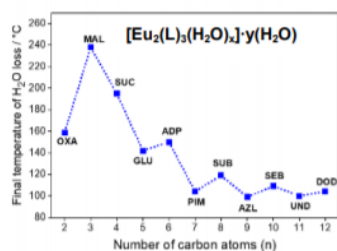


Fig. 1: Zigzag pattern obtained from final temperature (°C) of released H₂O molecules as a function of the number of carbon atoms ($2 \leq n \leq 12$).

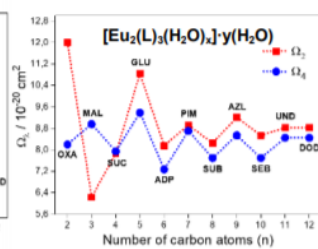


Fig. 2: Odd-even effect on the experimental intensity parameters Ω_2 (red squares) and Ω_4 (blue circles) as a function of the number of carbon atoms ($2 \leq n \leq 12$).

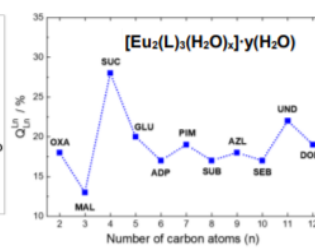


Fig. 3: The relationship between the emission intrinsic quantum yield (Q_{Ln}^{Ln}) as a function of the number of carbon atoms ($2 \leq n \leq 12$).

References:

[1] Moura Jr., R. T., Carneiro Neto, A. N., Longo, R. L., Malta, O. L., On the calculation and interpretation of covalency in the intensity parameters of 4f-4f transitions in Eu^{3+} complexes based on the chemical bond overlap polarizability. *J. Lumin.* 2016, 170, 420-430.

