

Lutetium(III) centered metallacages of the type $[\text{LuM}_2\text{L}_3]\text{NO}_3$ ($\text{M} = \text{Mn}^{2+}$, Cu^{2+} , and Zn^{2+} ; $\text{L} = 2,6\text{-dipicolinoylbis}(\text{N},\text{N}\text{-diethylthiourea})$)

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Metallacages containing multiple cations present interesting chemical features and may serve as a platform in nuclear medicine for incorporation of radionuclides used in imaging or therapy like ^{68}Ga and ^{177}Lu .^[1] In the present work, we report the synthesis and characterization of three new complexes that combine Lu^{3+} and M^{2+} ions from the first transition metal row with 2,6-dipicolinoylbis(*N,N*-diethylthiourea), H_2L , as ligand. The resulting in complexes of composition $[\text{LuM}_2(\text{L})_3]\text{NO}_3$, where $\text{M} = \text{Mn}^{2+}$, Cu^{2+} , and Zn^{2+} . The FTIR spectra of the complexes confirm the deprotonation of the ligands by the absence of the νNH , found at 3273 cm^{-1} in the spectrum of H_2L . The chelate formation is confirmed by the shifts of the $\nu\text{C}=\text{O}$ vibration from 1686 cm^{-1} in H_2L to approximately 1586 cm^{-1} in the complexes. The ESI mass spectra of the complexes show the expected molecular ion peaks for $[\text{M}]^+$. The composition of $[\text{LuM}_2(\text{L})_3]\text{NO}_3$ was also confirmed by the elemental analysis values. Furthermore, the $[\text{LuZn}_2(\text{L})_3]\text{NO}_3$ complex was characterized by single-crystal X-ray diffraction. The compound crystallizes in the monoclinic crystal system and $P2_1/c$ space group. Each Zn^{2+} center is coordinated to three sulfur and three oxygen donor atoms forming a distorted trigonal bipyramidal coordination sphere as shown in Figure 1. The Lu^{3+} center is coordinated to three nitrogen and six oxygen donor atoms and, consequently, shows a coordination number of nine and a tricapped trigonal prism polyhedron (see Figure 1). These products might have potential applications in nuclear medical procedures using the ^{177}Lu nuclide.

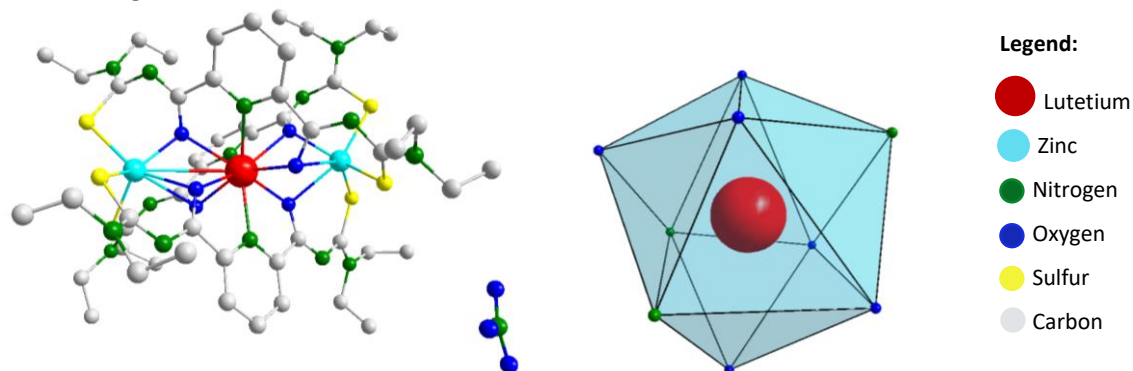


Figure 1: Molecular structure of $[\text{LuZn}_2(\text{L})_3]\text{NO}_3$ and the coordination polyhedron around the Lu^{3+} ion.

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References

[1] A. Baitullina *et al.*, *EJNMMI Radiopharmacy and Chemistry*, **8**, 40 (2023).