Two New Zinc(II) and Copper(II) Complexes Based on 1, 2, 4-Triazole Carboxylic Ligand

Catiúcia R. M. O. Matos[1](PG), Sérgio Pinheiro[2](PQ), Marcus P. F. Silva[2] (PG), Célia M. Ronconi*[1](PQ)

catiuciarmom@gmail.com and cmronconi@id.uff.br

[1]Laboratório de Química Supramolecular e Nanotecnologia and [2]Laboratório de Síntese Orgânica, Instituto de Química, Universidade Federal Fluminense, Campus do Valonguinho, CEP 24020-141 Niterói, RJ, Brazil.

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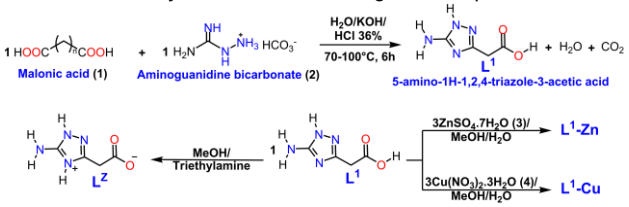
Introduction

Triazoles are extensively used in clinics and are promising owing to their antifungal, anticancer, and antibacterial properties.[1] To enhance the role of biological activities, several 1, 2, 4-triazole complexes based on bio-active metal have been designed as potential drugs due to DNA binding ability.[2] Copper and zinc(II) are known as essentials elements which are inserted in many biological processes, e.g., metalloproteins/enzymes active sites.[3] The anti-inflammatory activity of the 1, 2, 4-triazole **L[1]** was previously investigated and showed medium edema inhibition.[4] In this work we describe the syntheses and crystal structures of two zinc (II) and copper (II) complexes based on 1, 2, 4-triazole **L[1]** ligand.

Results and Discussion

The synthetic rout to obtain **L[1]**, **L[Z]** and the two complexes (**L[1]**-Zn and **L[1]**-Cu) is represented in the Scheme 1.

Scheme 1: The synthesis of the investigated compounds.



The nucleophilic addition of **2** to the protonated carbonyl **1** affords the **L[1]** in a yield of 15%.[4] Zinc (II) and copper (II) complexes were obtained by the addition of an aqueous solution of **3** and **4** to a methanol solution of **L[1]** under stirring. The **L[1]** and both complexes were characterized by single crystal X ray diffraction and ATR-IR. In addition, **L[1]** and **L[1]-Zn** were characterized by Raman spectroscopy, ^{1}H NMR and thermal analyses. The structural analyses show that **L[1]** crystallizes in the $P4_3$ space group as a zwitterion **L[Z]**, Figure 1(a). **L[1]-Zn** crystallizes in the $P2_1/n$ space group with two H_2O molecules in the axial position and two **L[1]** oppositely arranged forming a helical axis in the equatorial base. An octahedral geometry is observed for the Zn (II) center. The carboxylate group of **L[1]** coordinates in a monodentate mode and along with the coordination of N4 to Zn (II) results in a six-membered ring, Figure 1(b).

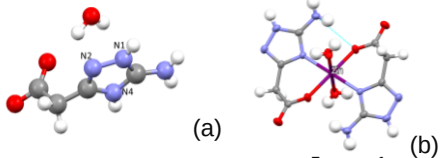


Figure 1. Structural representation of (a) **L[Z]**; (b) **L[1]-Zn**.

The **L[1]-Cu** crystallizes in a triclinic $P\bar{1}$ space group as a hydroxo-bridged tetranuclear copper(II) complex, Figure 2. The Cu2 center exhibits a distorted octahedral geometry and acts as a bridge connecting four subunits, Figure 2(b). Cu1 center has a distorted octahedral geometry, Cu3 an octahedral geometry and Cu4 a square pyramidal geometry, Figure 2(a). Jahn-Teller effect is present in this compound. The carboxylate group of **L[1]** coordinates in a monodentate mode and N1 and N2 coordinates to the different Cu (II) centers, while N4 is protonated and uncoordinated as was found for **L[Z]**.

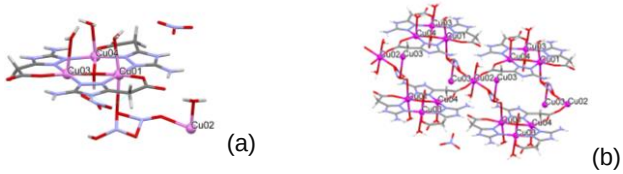


Figure 2. (a) Structure of the tetranuclear subunit. (b) Four subunits connected through Cu2 forming a discrete structure for **L[1]-Cu**.

Conclusions

We successfully obtained two new 1, 2, 4-triazole carboxylic complexes with different coordination modes for **L[1]** when coordinated to Cu(II) and Zn(II) metal centers.

Acknowledgments

CAPES, PPGQ-UFF, LAME, LAMATE, LDRX-UFF.

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