XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

New zinc complexes coordinated to catecholate ligands: chemical properties and antiviral activity

Ana Júlia G. Baviera [1], Evelyn C. S. Arantes[2], Natasha M. Cassani[3], Bruna C. Sandim[3], Ana Carolina G. Jardim[3], Renata G. de Lima[1,2]

[1]ICENP, Universidade Federal de Uberlândia, Ituiutaba/MG, Brazil.
[2]Instituto de Química (IQ), Universidade Federal de Uberlândia, Uberlândia/MG, Brazil.
[3]Laboratory of Antiviral Research, Universidade Federal de Uberlândia, Uberlândia/MG, Brazil.
E-mail: ana.baviera@ufu.br

Thematic Area: Biological Inorganic Chemistry

Keywords: Zinc (II) complexes, catecholate ligand, antiviral activity.

Biological trace metals, such as zinc, are essential to life and health of humans[1]. Several Zn(II) complexes have been recognized for their biological activities principally for preventive effects on infectious diseases and for low toxicity[2]. In this work, two Zn(II) complexes were synthesized, such as $[Zn^{II}Cl_2(bpy)(cat)]$ (1) and a binuclear $[Zn^{II}_2Cl_4(bpy)_2(dhb)]$ (2), where bpy = 2,2'-bipyridine, cat = catechol and dhb = 2,3-dihydroxybenzoic acid and evaluate antiviral activity against ZIKV (Table 1). For the synthesis, equimolar amounts of $ZnCl_2$ salt and ligand bpy were dissolved in methanol and added to catecholate ligand dissolved in methanol with pH = 14 adjusted with NaOH. After 1h of constant stirring at room temperature (≈ 30 ^{0}C) a yellow-green precipitate was formed. The precipitate formed was isolated and washed with portions of methanol, acetone, and ethyl ether. The elemental analysis reveals that the structural proposed for the complexes are consistent between theory and experimental values. The binuclear complex (2) was proposed based in the ^{1}H NMR and EM-MS analysis. In the complex (1), the zinc ion linked to diolate group, differently that complex (2) where for the Zn^{2+} coordinated to dhb ligand by diolate and carboxylate groups. The cathecolate ligands was stabilized after ion metal coordination in quinone state (C=O) for both (1) and (2) complexes analyzed by FTIR in compare to free ligands. The conductivity results contributed to the quinone oxidation state for both complexes, indicative of neutral ion complexes. Electronic absorption spectra for (1) and (2) were obtained in DMSO. The observed spectrum exhibits an absorption band at 284 nm (ε =1.55 x 10^4 L mol^{-1} cm^{-1}), corresponding to intra-ligand transition. The emission and excitation profiles were available for the complexes (1) and (2) showed under excitation at 280nm maximum emission at 320nm and 345nm respectively.

Table 1. Effect of zinc compounds on Vero E6 cells viability and ZIKV infectivity (%).

Compounds	Cell Viability (%)	Inhibition of ZIKV replication (%)
$[Zn^{II}Cl_2(bpy)(cat)]$ 10 µM	92.8	26.2
$[Zn^{II}_2Cl_4(bpy)_2(dhb)]$ 10 µM	94.5	31.1
$[Zn^{II}Cl_2(bpy)]$ 10 µM	87.1	19.2
catechol 2 µM	81.1	17.6
2,3-dihydroxybenzoic acid 2 µM	120.6	36.1

Acknowledgments: CNPq and Capes; RELAM-UFU.

References

[1] M. Jaya Brabha, *et al*. Chemical Physics Impact, **7**, 100248 (2023).
[2] K. Artur, *et al*. Archive of Biochemistry and Biophysics, **611**, 3-19 (2016).