Synthesis and Characterization of a New Synthetic Metallohydrolase for Catalysis and Biochemical Applications

Graciela A. S. Silva*[1] (PG), Ademir Neves[1] (PQ), Ebbe Nordlander[2] (PQ), Rosely A. Peralta[1] (PQ), *gra_qmk@hotmail.com
[1]*Universidade Federal de Santa Catarina – SC – UFSC*
[2]*Lunds Universitet - SE*

Keywords: *Bioinorganic Chemistry, Heterodinuclear Complex*

Introduction

The great structural complexity of metalloenzymes, such as PAPs, requires the use of low molecular weight compounds to help the understanding of the roles of metal ions in biological systems[1,2]. In this sense we present herein the synthesis and characterization of a new dinuclear complex as biomimetic for PAPs.

Results and Discussions

The ligand H_2L_1 was synthesized analogously to the literature.[2] The ligand H_2L_1 was characterized by infrared spectroscopy, IR (KBr) (cm^{-1}): ν (C-H_{ar} and C-H_{aliph}) 3050-2843; ν (C=O) 1682; ν (C=N and C=C) 1588-1469; ν (C-O) 1278; δ (C-H_{ar}) 750. It was also characterized by nuclear magnetic resonance (NMR) ^1H, δ_H in ppm (400 MHz; $CDCl_3$): 10,26 [1H, aldehyde], 8,54 [2H, py]; 8,43 [1H, py], 7,61-6,78 [11H, ar]; 3,86-3,71 [12H, CH_2], 3,05-2,96 [4H, CH_2], 2,23 [3H, CH_3]; 2,19 [3H, CH_3] and by mass spectrometry in CH_3OH and its isotopic species simulation signal with a *m/z* $[602.3126+H]^{+1}$.

An heterodinuclear complex with the core $[Fe^{III}(\mu\text{-}OH)Zn^{II}]$ was synthesized and characterized. The unsymmetric ligand coordinate to Zn^{II} with the soft side, and the hard side coordinate to the Fe^{III} ion.

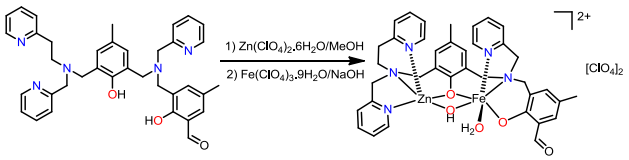

Figure 1. Synthesis of the complex

The complex was characterized by infrared spectroscopy, IR (KBr), (in cm^{-1}): ν (OH) 3443; ν (C-H_{ar} and C-H_{aliph}) 2916-2847; ν (C=N and C=C) 1604-1419; ν (C-O) 1264; δ (C-H_{ar}) 768.

Figure 2 shows the UV-Vis spectra obtained for the complex in acetonitrile. The spectrum of the complex shows two absorption bands, one at λ_{max}=513 nm (ε= 1971 $L.mol^{-1}.cm^{-1}$) and other at $\lambda_{máx}$=363 nm (ε= 7636 $L.mol^{-1}.cm^{-1}$) attributed with a charge transfer band (LMCT) phenolate→iron(III) pπ-dπ* and pπ-dσ*.

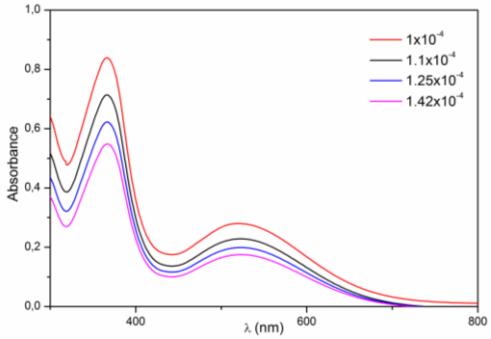

Figure 2. UV-Vis spectra for the complex.

It was also characterized by electrochemistry through cyclic voltammetry.

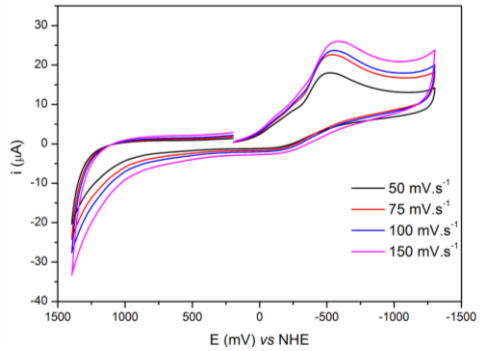

Figure 3. Cyclic voltammogram of the complex.

The redox character of the complex in EtOH/H_2O (70:30, %v/v) using KCl 0.1 $mol.L^{-1}$ at 25 °C. The redox character of the complex was analyzed at 50, 75, 100 and 150 $mV.s^{-1}$ with a process that can be attributed to the iron center, E_{pc}°= -545 mV, (pH 7.46).

Concluding Remarks

The ligand and complex were synthesized and characterized. However, it is still necessary to make new tests showing its catalytic activity against the 2,4-BDNPP substrate.

Acknowledgements

USFC, CAPES, STINT and INCT-catalise

[1] NEVES, A. et al. *J. Am. Chem. Soc.* **2007**, 129, 7486.
[2] MUXEL, A. et al. *Inorg. Chem.* **2014**, *53*, 2943.