

## In situ Synthesis of a Zwitterionic Ligand from 5,5'-Carbonylbis(2-benzofuran-1,3-dione) to Form a Co(II) Coordination Polymer

Thiago A. Grigolo<sup>1</sup> (IC), Sílvia D. de Campos<sup>1</sup> (PQ), Paula Brandão<sup>2</sup> (PQ), Elvio A. de Campos<sup>1\*</sup> (PQ).

\*elvioantonio@uol.com.br

<sup>1</sup> - Centro de Engenharias e Ciências Exatas, Unioeste, Rua da Faculdade 645, 85903-000, Toledo, PR, Brazil.

<sup>2</sup> - Departamento de Química, Universidade de Aveiro, Campus Santiago, 3810-193, Aveiro, Portugal.

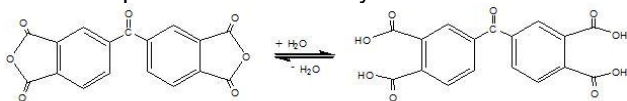
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### Introduction

The design and construction of self-assembled structures are current interest in the field of supramolecular chemistry and crystal engineering. One of the reasons for such interest is the possibility to generate materials with specific architectures and potential applications. Usually, it depends on the combination of some factors such as coordination geometry of metal ions, the nature of organic ligands and counterions, pH and sometimes the metal:ligand ratio.<sup>1</sup> Polycarboxylic aromatic acids have been widely used to construct high-dimensional structures with large pores or undulating layers.<sup>2</sup> The 3,3',4,4'-benzophenonetetracarboxylic acid is one of those acids that shows an interesting conformational variation depending of the pH.<sup>1</sup> On the other hand, diamines are a common class of compounds that can be used as an ordinary ligand in self assembled structures. In this work are presented the results of a hydrothermal synthesis of a Co(II) coordination polymer using two distinct ligand: an aromatic dicarboxylic acid and a diamine.

### Results and Discussion

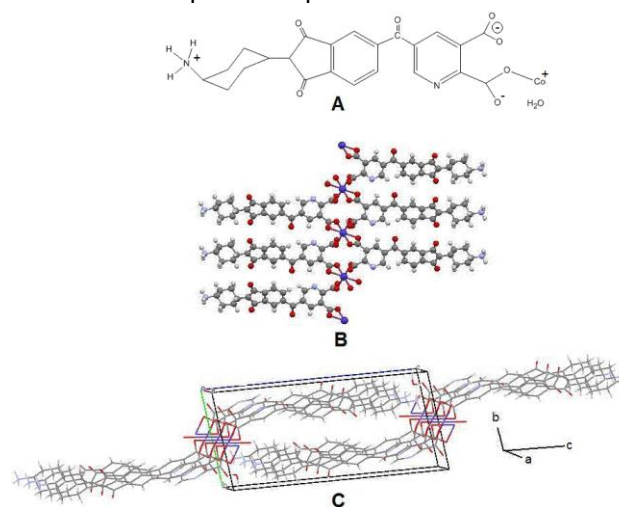
As source of the aromatic dicarboxylic acid it was utilized 5,5'-carbonylbis(2-benzofuran-1,3-dione) that after complete dissolution hydrolyses, Fig.1, gives the correspondent tetracarboxylic acid:



**Figure 1.** Hydrolysis of 5,5'-carbonylbis(2-benzofuran-1,3-dione).

The goal was to obtain layers of Co(II) coordinated to the polycarboxylic acid connected by diamine in a pillared structure. The basic hydrolysis performed in presence of the diamine led to the correspondent carboxylate anion that can coordinate to the metal ion. The synthesis procedure consisted in the dissolution of 0,50 mmol of 5,5'-carbonylbis(2-benzofuran-1,3-dione) in 15 mL of an aqueous solution of 0,50 mmol of 1,4-cyclohexanediamine that was stirred for 1 h followed by addition of 0,25 mmol of aqueous CoCl<sub>2</sub> solution. The pH was adjusted with 10% Na<sub>2</sub>CO<sub>3</sub> solution and then the mixture was transferred to a Teflon lined stainless steel reactor and heated at 180° C for 24 h. The pale

orange reddish crystals were collected and the crystalline structure was determined, Fig.2, by single crystal X ray diffraction and confirmed by infrared and <sup>13</sup>C NMR spectroscopies.



**Figure 2.** Representation of Co(II) coordination polymer with the zwitterion ligand (A) monomeric unit structure, (B) single Co(II) octahedral layer viewed along b\* axis and (C) ORTEP diagram showing the interpenetrating layers and the channel along "a".

The triclinic structure from space group P -1 (a = 5.8624(7); b = 9.1815(11); c = 19.916(2); α = 83.927(3); β = 88.007(3) and γ = 78.591(3)) presents negative charge on Co(II) region while the extremities of the chains are positively charged. The crystal structure is stabilized by a H<sub>2</sub>O molecule.

### Conclusion

Reaction between 5,5'-carbonylbis(2-benzofuran-1,3-dione) and 1,4-cyclohexanediamine in a specific pH yields the coordination polymer [C<sub>23</sub>H<sub>19</sub>O<sub>7</sub>N<sub>2</sub>Co.H<sub>2</sub>O]<sub>n</sub>. Moreover, its crystal structure was determined by appropriate analysis and the resulting solid presents a new zwitterion ligand.

### Acknowledgments

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