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XAFS studies of copper complexes with coumarin acid derivatives

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Keywords: coumarin, coumarin acid derivatives, copper, XAFS

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Coumarins represent an important type of *O*-donor heterocycles with typical benzopyrone framework. The natural as well as synthetic coumarins, have a large spectrum of biological activity. Such derivatives proved its usefulness as anti-coagulants [1], antibacterial agents [2], antifungal agents/medicines [3], biological inhibitors [4], chemotherapeutics [5] and as bio-analytical reagents [6]. It has been found out that coordination of metal ions to therapeutic agents (such as simple coumarins) can improve their efficacy and accelerate bioactivity [7]. In many cases such metal complexes are more potent and less toxic comparing to the parent drug. Therefore, among others, also biologically active metal complexes of coumarin based ligands are being widely investigated. There are some reports about biological activity of coumarin acids complexes, however, among reports about biological activity there is very little information concerning metal organic ligand binding mechanism.

Such situation is caused mainly due to lack of experimental techniques which allows to study compounds which do not have long range order in its structure. X-ray absorption fine structure (XAFS) technique already proved its usefulness in similar studies [7] and was applied in this case. The great advantage of XAS is that it can be used for crystal as well as amorphous materials.

The XAFS measurements were performed at Cu K-edge at XAFS beamline at Elettra (Trieste, Italy). Complexes were investigated in both powder and liquid form. For the complexes in the form of microcrystalline powder the transmission detection mode was used, whereas for liquid samples (which concentration was in the mmol range) the fluorescence detection mode was required and applied.

In order to find out whether chemical method used for obtaining complexes introduces some structural changes, powder samples were synthesized using two methods: direct and electrochemical. In order to obtain liquid samples, the dimethyl sulfoxide (DMSO) and dimethylformamide (DMF) were used as solvents. Both of them are popular organic solvents used during the synthesis of such compounds and are commonly used for crystallization of Cu complexes. Moreover, DMSO is most often used (as it was in our case) during microbiological activity tests procedures. It is possible that the molecules of solvents can modify the coordination sphere of metal cation and therefore modify the properties of studied complexes.

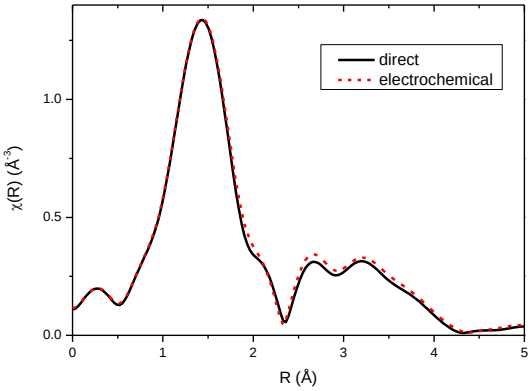

Figure 1. Comparison of the FT EXAFS oscillations for one of the powder compounds obtained using direct (black solid line) and electrochemical (red dotted line) method.

We plan to show and discuss the structural results obtained for powder and liquid form of Cu complexes with coumarin acid derivatives.

Acknowledgments: Experimental research was funded from the Polish National Science Centre (Grant No. UMO-2012/07/D/ST5/02251). This research was supported in part by PL-Grid Infrastructure. Financial support from the EU FP7 EAgLE project under the grant agreement REGPOT-CT-2013-316014 is gratefully acknowledged.

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