P-20

Structural study of the Cu complexes with benzofuran derivatives

D. Kalinowska[1]*, A. Wolska [1], M. T. Klepka [1], A. Drzewiecka-Antonik [1], K. Ostrowska[2] and M. Struga[2]

[1]*Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland,*
[2]*Medical University of Warsaw, Żwirki i Wigury 61, 02-091 Warsaw, Poland*

Keywords: benzofuran derivatives, copper, XAFS, FTIR spectroscopy

*e-mail: diana.kalinowska@ifpan.edu.pl

The derivatives of benzofuran (heterocyclic compounds consisting of fused benzene and furan ring) are important group among biologically active compounds. A broad spectrum of biological activities, such as antimicrobial (antifungal and antibacterial), antiviral, anti-inflammatory, antitumor, antihyperglycemic, analgesic or antipyretic make the complexes of benzofuran derivatives with metal ions perfect as potential pharmacological agents [1–5].

Copper is an essential element of a living organism. As a critical component of enzymes and proteins it plays an important role in biological processes [1]. Copper complexes are very effective anti-inflammatory agents. They also demonstrate considerable potential in the treatment of chronic diseases, including gastric ulcers and bowel disease, epilepsy, cancer and diabetes [5]. Knowledge of their structure is extremely important in the planning of chemical reaction, intended to obtain the compounds of the assumed physical and chemical properties. However, quite often it is impossible to obtain a complex in a crystalline form. Therefore, the X-ray absorption fine structure (XAFS) technique was implemented. The great advantage of XAFS is that it can be used for amorphous materials as well as for crystals. XAFS analysis provides information about atom's local environment (the coordination number, the distance from metal to neighboring atoms) and information about relative structural disorder.

As ligands for the complexation reaction the derivatives of benzo[b]furan were used. FTIR spectroscopy was used for monitoring the complexation reactions and for identifications of possible coordinating group to the metallic center. Due to fact that XAFS analysis requires initial model Cambridge Structural Database (CSD) was searched for it.

XAS measurements at Cu K-edge were performed at CEMO beamline at DESY (Hamburg). The samples in a form of powder were pressed into a carbon tape. Spectra were collected at liquid nitrogen temperature using transmission detection mode. EXAFS analysis was performed using the Athena and Artemis programs based on the IFEFFIT library of numerical XAFS algorithms [6].

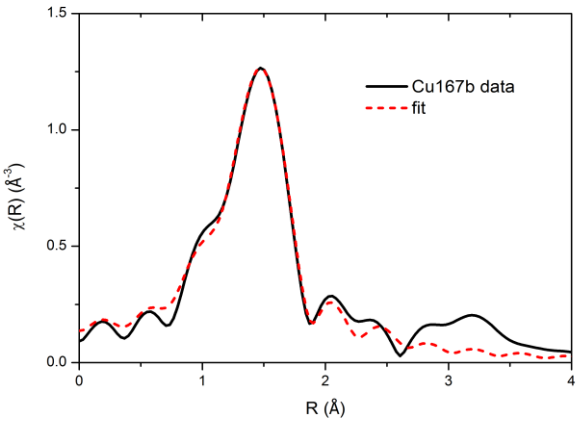

Figure 1. FT EXAFS oscillations for one of the investigated complexes (black solid line) and fitting result (red dotted line).

The EXAFS analysis revealed that the first coordination sphere is composed only from oxygen atoms and depending on the complex their quantity differs. Structural details obtained from the analysis will be discussed on the presentation.

[1] A. Drzewiecka, A. E. Kozioł, M. T. Klepka, A. Wolska, H. Przybylińska, S. B. Jimenez-Pulido, K. Ostrowska, M. Struga, J. Kossakowski, T. Lis, *Polyhedron* **43** (2012) 71.
[2] A. Drzewiecka, *Struktura potencjalnych ligandów O-donorowych i ich kompleksów organicznych z jonami metali* (Lublin, 2010).
[3] H. Khanam, Shamsuzzaman, *Eur. J. Med. Chem*, **97** (2015) 483.
[4] A. Radadiya, A. Shah, *Eur. J. Med. Chem*, **97** (2015) 356.
[5] G. Cerchiavo, A. M. da Costa Ferreira, *J. Braz. Chem. Soc*, **17** (2006).
[6] B. Ravel, M. Newville, *J. Synch. Rad.* **12** (2005) 537.