IO-01 **Sun. 15. 06., 18^{40}-19^{00}**

XAFS study of the Ni complexes with hydantoin derivatives

A. Wolska[1]*, M. T. Klepka[1], A. Drzewiecka-Antonik[1], M. Puszynska-Tuszkanow[2] and M. Cieslak-Golonka[2]

[1]*Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*
[2] *Faculty of Chemistry, Wroclaw University of Technology, 27 Wybrzeze Wyspianskiego, 50-370 Wroclaw, Poland*

Keywords: metal-organic complexes, XANES, EXAFS, synchrotron radiation

*e-mail: Anna.Wolska@ifpan.edu.pl

Studies on parent hydantoin and its various derivatives are of fundamental and practical importance due to their physiological action as anticonvulsant, antiepileptic, anti-inflammatory and anticancer drugs [1]. Recently, the potential applications of compounds containing a hydantoin fragment for HIV-1 treatment has also been suggested [2]. Among newly synthesized transition metal complexes some exhibit activity against human cancer cell lines MCF-7 (breast adenocarcinoma) and A549 (non-small cell lung carcinoma) as well as mouse fibroblasts cell line (BALB/3T3) [3]. The cytotoxity data indicate that the antitumor activity of coordination compounds are modulated by many factors like e.g. the nature of the alkyl group substituted to the heterocyclic ligands, the hydrogen bond pattern, type of metal or/and environment around metal cation. Hydantoins are promising ligands to obtain metal-based compounds with anticancer activity due to different ways of binding to the central metal ion [4].

The metal complexation reaction usually modifies the biological activity of a ligand [5]. Since the biological properties of the compound are directly related to its structure, the study on metal-binding ability of hydantoin derivatives is necessary. The X-ray absorption fine structure spectroscopy (XAFS) technique is perfect for this task since it can provide information about local atomic neighborhood and coordination polyhedra around metal cations regardless of the state or crystallographic form of the investigated material. This is especially important for structural studies of compounds without long range order like in this case.

The Ni(II) ions with *N,O*-donor hydantoins in the novel biologically active complexes were studied. The XAFS measurements at Ni K edge were performed at I811 beamline at MAX-LAB. Both, extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES), regions were analysed. EXAFS analysis provided information about the average coordination number, the type of coordination atoms, their distance from the metal cation and relative structural disorder. The shape of a XANES spectrum strongly depends on the angles between the neighboring atoms, therefore, theoretical calculations based on the model proposed from EXAFS analysis allowed to determine the 3d arrangement around the absorbing atoms.

Acknowledgments: The synchrotron experiment was partially supported by the Baltic Science Link project coordinated by the Swedish Research Council, VR.

[1] S.S. Block, *Disinfection, Sterilization and Preservation*, 4th-ed., (Lea & Febiger, Philadelphia, **2003**).
[2] R. Vardanyan, H.J. Hruby, *Synthesis of Essential Drugs*, Elsevier, **2006**.
[3] M. Puszyńska-Tuszkanow, T. Grabowski, M. Daszkiewicz, J. Wietrzyk, B. Filip, G. Maciejewska, M. Cieślak-Golonka, *J. Inorg. Biochem*. **105** (2011) 17.
[4] M. Puszyńska-Tuszkanow, M. Daszkiewicz, G. Maciejewska, Z. Staszak, J. Wietrzyk, B. Filip, M. Cieślak-Golonka, *Polyhedron* **30** (2011) 2016.
[5] G. Maciejewska, W. Zierkiewicz, A. Adach, M. Kopacz, I. Zapała, I. Bulik, M. Cieślak-Golonka, T. Grabowski, J. Wietrzyk, *J. Inorg. Biochem*. **103** (2009) 1189.