

SEMINARIUM RENTGENOWSKIE

Dnia 17.10.2017r. o godz. 10.30, w sali D Instytutu Fizyki PAN, odbędzie się seminarium rtg., na którym mgr **Diana Kalinowska** z IF PAN, wygłosi referat na temat:

„Molecular structure investigation of coumarin complexes with Cu ions”

Streszczenie:

In the presented study determination of the binding mechanism between metal ion and organic ligand in two copper complexes with coumarin derivatives is shown. Coumarin is known for its wide range of biological activity (e.g. anti-inflammatory, antibacterial or cytotoxic [1]) and therefore it can be used as a scaffolding in the design of synthetic compounds that exhibit extensive pharmacological activity.

Both presented complexes exhibit selective activity against gram-positive bacteria. Unfortunately, obtaining these compounds in a crystalline form did not succeed. Therefore, to determine the geometry of complexes X-ray Absorption Spectroscopy (XAS) technique was applied. This method gives information about the local structure around the specific element and is ideal to study compounds regardless of their crystal form or state [2–3].

Measurements were performed at Cu K-edge (8979 eV) at XAFS beamline of the Elettra storage ring (Trieste, Italy). The XAS spectra were collected in transmission mode for powdered samples. Reference oxides were also measured. To gather structural information about copper complexes, both near edge structure (XANES) and extended fine structure (EXAFS) have been analyzed. Obtained information have been used to construct model which have been further analyzed to describe molecular structure of the investigated compounds. Additionally, DFT calculations and XANES simulations have been performed.

Described structural studies on the coumarin copper complexes provided detailed information about coordination geometry of copper cations in studied compounds.

Prof. dr hab. Krystyna Jabłońska