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Structural studies of metal-organic ligand complexes using X-ray absorption spectroscopy

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The discovery that the metal complexes, especially with transition metals like copper and silver, can be more effective than the parent ligands opened a new field of drug research. In our laboratory the synthesis and structural characterization of novel biologically active metal-organic ligand complexes is carried out.

The direct, hydrothermal and electrochemical synthesis are used for complexation reactions. New compounds (copper and silver complexes) are tested for microbiological activity on standard and clinical strains of fungi and bacteria. The use of the microorganisms taken from patients is an important stage of our studies. As a result of the civilization development and the various human activities (e.g. inappropriate use of antibiotics) the mutation of infecting cells of bacteria and fungi is observed. We want to face this problem and obtain metal-based complexes with high selectivity and efficacy.

The synthesized compounds are initially characterized by elemental analysis, IR and UV-VIS spectroscopies. More detailed information about the coordination sphere of bioactive complexes is obtained by applying the X-ray absorption spectroscopy. Extended X-ray absorption fine structure (EXAFS) analysis provides information about the average coordination number, the type of atoms around the metal ion and the distances between the metal center and the coordinating molecules. This data allows proposing a coordination mode of ligands to the metal cation in the studied complexes. From XANES spectra (X-ray absorption near edge structure) it is possible to determine the oxidation state of the metal in the analyzed compounds. In addition, by taking advantage of the fact that the shape of XANES spectra strongly depend on the angles between central and neighboring atoms, the analysis of these spectra allow confirmation and improvement of the coordination modes proposed from the EXAFS analysis.

Moreover, the density functional theory level calculations are carried out. The theoretical study on metal complexes (geometry optimization, calculations of vibrational frequencies, simulations of UV-Vis spectra etc.) complements the experimental data.

During presentation the structural studies on complexes with derivatives of coumarin (*O*-donor ligands) and derivatives of thiourea (*N*,*S*-donor ligands) will be presented.

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