L-14 **Session B, Wednesday, 15.06., 9^{00} - 9^{40}**

Structural studies of bioactive metal-organic ligand complexes using XAFS

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Biologically active metal complexes of organic ligands are being widely investigated. However, very often among reports about biological activity there is little information concerning metal – organic ligand binding mechanism. This lack is a result of a fact that for coordination compounds it is difficult to obtain crystals. In such a case diffraction techniques are inapplicable and any structural information can only be speculated. Detailed knowledge about structure is extremely important in studies of bioactive coordination complexes. Without it planning the chemical reactions to properly modify chemical or physical properties of final product is ineffective.

X-ray absorption fine structure (XAFS) technique is not commonly applied to study metal-organic ligand interactions. The great advantage of XAFS over other experimental techniques is that it can be used for crystal as well as amorphous materials at different states: (i) solid, (ii) liquid or (iii) gaseous. XAFS provides information about the local atomic order, coordination number, kind of atoms, oxidation state, relative disorder and even angles between central atom and near neighbours. Such information is essential to study structure-activity relationship for the disordered complexes.

Goal of our studies is to get information about binding mechanism of organic ligand to metallic center. In order to achieve that we perform analysis in several steps. First, infrared spectroscopy is used to monitor whether complexation reaction was successful. In parallel elemental and thermal analyses are being performed. In the second step Cambridge Structural Database (CSD) is being searched to find initial model for DFT calculations and EXAFS analysis. Third step is refining model using XANES analysis. The last step is confirmation of the final model using EXAFS analysis.

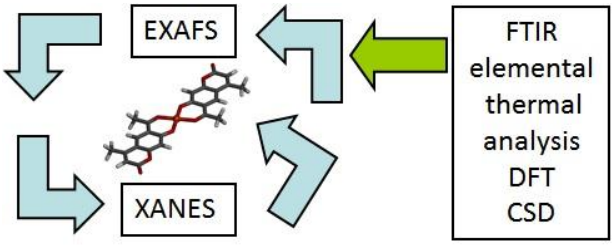

Figure 1. Scheme of the analysis steps

During presentation examples of performed studies with e.g.:

(i) phenoxyacetic and benzoic acids [1],
(ii) benzo[*b*]furan derivatives [2],
(iii) methylohydantoin [3],
(iv) coumarin derivatives [4]

and future perspectives will be presented and discussed.

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