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X-ray absorption spectroscopy – tool to resolve structure

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X-ray absorption fine structure (XAFS) spectroscopy is a powerful spectroscopic technique that attracts attention of scientists from many different fields. Development of new generation synchrotron sources and theoretical tools opened the potential of XAFS not only to the physicists but also to the chemists, biologists, engineers and others.

X-ray diffraction (XRD) provides information only about crystalline part of investigated materials. However, there are materials with high disorder or amorphous fraction where classical methods are insufficient and another tool is needed. In many cases XAFS can offer desired information.

XAFS uses X-rays from a synchrotron source for probing the structure of a matter at local atomic scale around almost any element in the periodic table (except the lightest). Main advantages of the XAFS are the elemental selectivity and sensitivity. Moreover, the measurements can be performed regardless the physical state of the investigated material. XAFS is usually being divided into two regions: X-ray Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS).

XANES directly probes the angular momentum of the unoccupied electronic states what provides information about the chemical bonding of the element [1-3]. The energy position of the edge can be treated as a fingerprint of the oxidation state of the absorbing atom.

EXAFS oscillations are used to determine the kind of elements, distances and the number of the atoms in coordination spheres around the investigated element [4].

During presentation results obtained for different kind of materials like natural minerals e.g. ilmenites, and metal-organic ligand complexes, with pharmacological potential will be discussed. Complementarity of the XAFS to the XRD studies will be shown.

Ilmenites are naturally occurring minerals used industrially to obtain white pigment. In order to optimize production process the knowledge about the minor and major phases present in an ore is essential. Standard procedure includes X-ray fluorescence (XRF), XRD or electron probe micro analysis (EPMA). However, these techniques occurred to be not sensitive enough particularly for minor phases and elements. To solve this problem XANES, together with linear combination analysis LCA, was used. Such approach allowed to identify and estimate content of the phases in an ilmenite ore [5].

Several examples of the metal-organic ligand complexes will be also discussed. Interest in such compounds is due to a fact that complexes demonstrate enhanced biological activity in comparison to parent organic ligand. However, in case of such compounds the main difficulty is to obtain single crystals for diffraction studies. To find the metal coordination sphere of non-crystalline compounds the XAFS can be applied. The combination of EXAFS and XANES techniques can provide detail information about metal-organic ligand interactions.

Examples of metal complex with: (*i*) hydroxybenzo[*b*]furan, (*ii*) benzo[*b*]furancarboxylic acid, (*iii*) benzoic acid, (*iv*) phenoxyacetic acid, (*v*) cinnamic acid will be shown [6].

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