XAFS studies of non-crystalline metal-organic ligand complexes

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Metal-organic ligand complexes are being widely investigated mostly due to fact that they usually exhibit higher biological activity and lower toxicity in comparison to free ligand. Among reports about the activity of complexes there is still insufficient information concerning metal-organic ligand binding mechanism. In particular it concerns complexes which were not obtained in a crystalline form. In such a case diffraction techniques are inapplicable and structural information can rather be speculated than experimentally determined. Due to their bioactive properties, a detailed knowledge about structure of these coordination compounds is extremely important.

In order to resolve molecular structure of the metal-organic ligand complexes in the non-crystalline state we have developed the methodology which is a combination of XAFS, elemental analysis, infrared and electronic spectroscopies (FT-IR, UV-VIS) and theoretical calculations performed at DFT level. Our methodology has been successfully applied to describe molecular structure of various bioactive Cu(II) complexes with hydroxycoumarins derivatives [1-3]. The microbiological activity for some of the studied complexes are comparable with commercially available drugs.

During presentation detailed information about methodology itself and results obtained for complexes of Cu(II) and Ag(I) with coumarin acids derivatives will be discussed.

References:

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