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XANES as a tool for determining a 3-D arrangement around the metal ions in the bioactive complexes

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The metal–organic ligand complexes came into close attention while it was discovered that through the complexation process one can obtain the metal-organic compounds with improved properties in respect to the parent ligand [1]. Since the properties of a compound depend on its structure, it is important to determine the geometry of the complex.

The shape of a spectrum in the XANES region strongly depends on the angles between the neighboring atoms. Therefore, XANES analysis can be used as a tool for determining the 3-D arrangement around the absorbing atoms. As an example the search of the neighborhood of the metal ions in Co(II) and Cu(II) complexes of cinnamic acid is shown.

The analysis is carried out as follows: (*i*) the EXAFS analysis is performed; (*ii*) from the structural database several models are selected with parameters being in agreement with the EXAFS results; (*iii*) for these models the XANES spectra are calculated with FEFF 9.5 code [2] and the best models are selected for the next step; (*iv*) the ligands in the models are rotated; (*v*) the best results are selected and checked again with the EXAFS results.

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