XAFS STUDY OF NOVEL TYPE OF METALLOCHELATES OF PHENYLAZODERIVATIVES OF SCHIFF BASES

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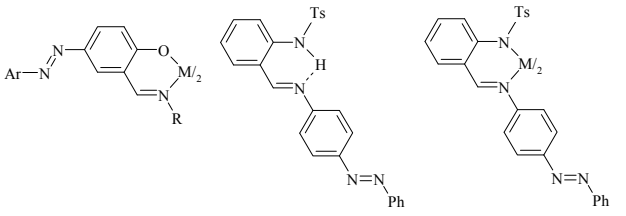
Acyclic and cyclic Schiff bases are the very important ligands of the modern coordination chemistry due to the possibility of creation on their basis novel polyfunctional materials: magnetics, luminophores, bioactive chelates, chemosensors and liquid crystals. Metallocomplexes of Schiff bases take an important place in supra- and nanochemistry [1,2].

Coordination compounds of Schiff bases with azogroup are represented by complexes of the ligands containing Ar-N=N- fragment in aldehyde moiety – chelates of azomethines of arylazosalicylaldehyde **1**. Schiff base derived from *o*-tosylaminobenzaldehyde and *p*-aminoazobenzene **2** and its metallochelates (Co2+, Ni2+, Cu2+) **3** were synthesized and investigated by XANES and EXAFS spectroscopy.



1 **2** **3**: M = Co (a), Ni (b), Cu (c), Zn (d)

The Ni*K*-, Co*K*- and Cu*K*-edges EXAFS spectra for the complexes were obtained at the Station K1.3b "Structural Materials Science" of the Kurchatov Center for Synchrotron Radiation and Nanotechnology (KCSRNT, Moscow, Russia). EXAFS data were analyzed using the IFEFFIT 1.2.11 data analysis package. The structural parameters, including interatomic distances (R), coordination numbers (CN) and the distance mean-square deviation- Debye–Waller factors (σ^2), were found by the non-linear fit of theoretical spectra to experimental ones. Experimental data were simulated using theoretical EXAFS amplitude and phase functions, which were calculated using the program FEFF7. The *modules* of Fourier transforms (MFT) of the Ni*K*-, Co*K*- and Cu*K*-edges EXAFS data for the metallochelates **3** are shown in Fig. 1. From our EXAFS and XANES analysis, it is possible to propose a model of coordination environment of Cu, Ni and Co ions in metallochelates **3**. All complexes possess distorted tetrahedral (due to additional coordination of oxygen atoms of Ts-tosylamino group) donor environment. The obtained distanses M…O(Ts) are dependent on the metal atom type so that Cu…O(Ts)< Ni…O(Ts)< Co…O(Ts).

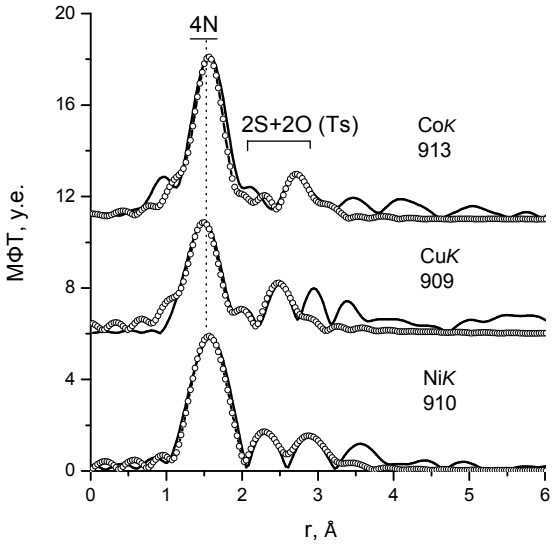


Figure 1. MFT of the Co, Cu and Ni*K*-edge EXAFS spectra for the metallochelates studied: experiment (solid lines) and best-fits (open circles).

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