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XAFS technique used to obtain structural information for complexes of coumarin derivatives with Cu

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The coumarin and its derivatives occur naturally in plants with therapeutic effect and have been used in natural medicine as traditional remedies [1]. Moreover, natural as well as synthetic coumarin derivatives have a large spectrum of biological activity and are widely investigated. Simple coumarins vary greatly in their molecular structure and this can influence their pharmaceutical properties [2,3]. Type and strength of their biological action usually depend on the number and kind of small substituents, namely hydroxyl or methoxy group. In general, it could be noticed that coordination of metal ions to therapeutic agents improves their efficacy and accelerates their bioactivity.

Electrochemically obtained Cu complexes with hydroxy derivatives of 4-methylcoumarin were structurally investigated using X-ray absorption fine structure spectroscopy (XAFS). Measurements at Cu K edge in the transmission detection mode were performed at I811 beamline at MAX-LAB.

Analysis of the extended X-ray absorption fine structure (EXAFS) provided information about the average coordination number, the type of coordination atoms, their distance from the metal cation and the relative structural disorder. It was discovered that the first coordination sphere is formed of 4 oxygen atoms for all investigated complexes. The Cu–O bond distances were estimated to be around 1.94(1) Å.

Using structural information obtained from the EXAFS analysis, the most probable models from Cambridge Structural Database (CSD) were selected and were used as the initial models in the X-ray absorption near edge structure (XANES) analysis. The shape of a XANES spectrum, in opposition to EXAFS, strongly depends on the angles between the neighboring atoms. Therefore, by performing calculation for models with different angular arrangement of the ligands, it was possible to propose and verify coordination polyhedra of all analyzed complexes.

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