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XAFS, FTIR, UV-Vis and DFT studies on Cu(II) complexes with coumarin derivatives

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Coumarin derivatives are an important pharmacophore present in numerous compounds, which can be isolated from natural sources. They show wide range of biological activity, such as antibacterial, anitiviral and anticancer [1]. Cu complexes are reported to show the enhancement of pharmacological activity in comparison to parent ligand, combined with lower toxicity [2]. Therefore study on Cu(II) complexes with coumarins are particularly interesting. Structural characterization of Cu(II) complexes with perspective pharmaceutical applications are essential for the understanding of structure-activity relationship [3].

The Cu(II) complexes with acetyl derivatives of 7-hydroxy-4-methylcoumarin have been synthesized electrochemically. These compounds were consequently characterized by several spectroscopic techniques.

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. The extended X-ray absorption fine structure (EXAFS) provided information about the coordination number and bond length in the first coordination sphere of Cu(II) ions. Further structural information was obtained from the X-ray absorption near edge structure (XANES) analysis. Studied compounds were also characterized in our laboratory by means of Fourier transform infrared (FTIR) and ultraviolet-visible (UV-Vis) spectroscopies. Consequently, the density functional theory level calculations were performed on preliminary structural models in order to and to facilitate the interpretation of spectroscopic data.

Our study shows that combination of spectroscopic and computational techniques enables structural characterization of studied compounds in lack of crystallographic data.

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