

## Structural studies of bioactive Ag(I) complexes with coumarin derivatives

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Silver complexes with organic ligands has been attracting wide attention due to their strong bactericidal properties. Among them those with coumarin derivatives since the coumarin core is a common structural motif in both natural products and bioactive molecules. Moreover, depending on the substituents around the cyclic core, coumarin-containing compounds have shown a wide range of pharmacological activity. Following this, two new Ag(I) complexes with coumaric carboxylic acid derivatives have been synthesized and structurally characterized.

Structural characterization of the complexes was conducted for noncrystalline materials

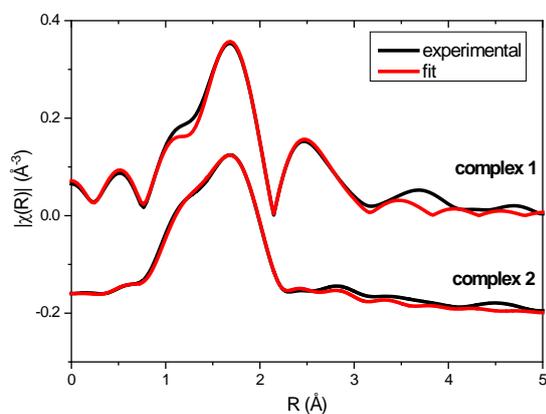


Figure 1 EXAFS fitting of the experimental oscillations (black line) and the fitting result (red line) for complex 1 and 2.

using a methodology developed by the authors<sup>1</sup>, which combines laboratory and synchrotron based techniques as well as density functional theory (DFT) calculations. The elemental analysis and attenuated total reflectance infrared (ATR-IR) spectroscopy provided information on the functional groups coordinating to the metal cation and the metal-to-ligand ratio. Extended X-ray absorption fine structure (EXAFS) spectroscopy supplied information about the coordination number and the kind of species surrounding the absorbing cation. X-ray absorption near edge structure (XANES) spectroscopy and DFT calculations helped to determine the most probable structural models.

In both complexes different coordination modes of carboxylate ligands were detected. For the Ag(I) complex with 4-oxo-4H-1-benzopyran-2-carboxylic acid (complex 1), carboxylate bridges was observed. For the complex 2, with 2-oxo-2H-1-benzopyran-3-carboxylic acid, a bidentate chelating motif was found. Moreover, the carbonyl oxygen atom of the coumarin ring coordinates to the silver cation in complex 2, while it is inactive in complex 1.

Additionally, microbiological activity of the investigated complexes was performed<sup>2</sup>. The complexes show activity against selected bacteria as well as *Candida* yeast. This activity is slightly lower for bacteria and the same or higher for *Candida* in relation to the reference substances: ciprofloxacin or fluconazole.

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### References

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