

## Abstract

Coordination complexes are one of the subjects of study of contemporary inorganic chemistry, also, a considerable interest has arisen in the development and synthesis of new coordination compounds possessing various biological activities, such as antimicrobial, anti-inflammatory, antifungal, antioxidant and anticancer;

For this purpose, we have synthesized in this work, six new original compounds based on sulfamethoxazole ligand: four mononuclear complexes with zinc, copper and cobalt, also, two polymers based on cobalt and silver metals;

The crystal structures of the latter were determined from low temperature x-ray diffraction data, they are characterized by preliminary analysis and by means of IR plus UV-Vis, accomplished by studying hydrogen bond networks and Hirshfeld surface analysis.

The in-vitro antibacterial/antifungal activities of the free ligand (SMX) and its zinc and copper complexes were evaluated using the well- diffusion method in DMSO (dimethyl sulfoxide). *Cotrimoxale* is used as positive control to make meaningful comparison.

In order to improve the understanding of the structure of coordination complexes, an entire calculation was performed in this study using the density functional theory DFT with the mPW1PW91 basis at the TZVP level of theory. Gaussian 03W and Gauss View 5.0.8 programs were utilized to achieve calculations and for structural and spectroscopic illustrations, respectively.

**Key words:** Single crystal, X-rays diffraction, Sulfamethoxazole, Transition metals, Hirshfeld surface analysis, Antibacterial/antifungal activities, DFT/mPW1PW91/TZVP method.