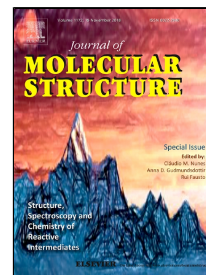


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# Synthesis, spectroscopic studies, X-ray powder diffraction data and biological activity of mixed transition metal complexes with oxalato and theophylline ligands

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## Abstract

The new series of divalent metal complexes  $[M(ox)(thy)_2]$ ;  $M = Cd^{2+}$ ,  $Ni^{2+}$ ,  $Mn^{2+}$ ,  $Fe^{2+}$ ,  $Cu^{2+}$  and  $Zn^{2+}$ , with mixed ligands oxalato (ox) and theophylline (thy) were prepared and characterized by molar conductance, FT-IR, UV-visible,  $^1H$  and  $^{13}C$  NMR and X-ray structure analysis. The crystal structure including the positions of the Zn (II) complex was determined by powder diffraction analysis using the FOX program. In the structure of zinc complex, the zinc (II) cations are octahedrally coordinated by two terminals N-bonding for theophylline ligand and by the O atoms of two oxalato bidentate ligand, resulting in discrete and slightly distorted octahedral complex. This complex was crystallized in the monoclinic system (C1 2/c1) space group and the unit cell parameters are  $a=11.8364(1)\text{\AA}$ ,  $b=4.5200(1)\text{\AA}$ ,  $c=9.9942(1)\text{\AA}$  with  $\beta$  ( $^\circ$ )= $126.4770(2)^\circ$ . The antimicrobial activity of the complexes was studied and the results of their tests show that the metal (II) complexes are more effective against several of bacterial and fungal strains.

**Keywords:** Mixed ligand; Complexes; Spectroscopy; X-ray structure; Molar conductance; Antimicrobial activity.

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