Cu(II) and Zn(II) complexes from a thiosemicarbazone derivative: Investigating the intermolecular interactions, crystal structures and cytotoxicity

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Abstract

Two complexes of Cu(II) and Zn(II) were prepared from a thiosemicarbazone derivative (H₂esct) using their corresponding metal acetates and 2,2'-bipyridine as base. The complexes were characterized by elemental analyses, UV-visible, FT-IR and NMR spectroscopy. The structure of the thiosemicarbazone derivative and its five coordinated complexes were also determined by the single crystal X-ray diffraction study. Copper complex got crystallized in triclinic $P\bar{1}$ space group and zinc complex in monoclinic $P2_1/c$ space group. The crystal structures of the complexes exhibited different types of intermolecular interactions, which have been further analyzed by Hirshfeld surface analysis and fingerprint plots. The *in vitro* cytotoxicity against Dalton lymphoma ascites cell lines showed that the Zn(II) and Cu(II) complexes are more cytotoxic than their corresponding proligands.

Keywords: Cu(II) complex, Zn(II) complex, Hirshfeld surface, Cytotoxicity

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