

STRUCTURAL, SUPRAMOLECULAR AND PHOTOLUMINESCENT PROPERTIES OF ONE-DIMENSIONAL Zn(II) AND Cd(II) COORDINATION POLYMERS BASED ON 2,6-DIACETYLPIRIDINE BIS(ISONICOTINOYLHYDRAZONE)

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Abstract. Two new one-dimensional coordination polymers: $\{[\text{Zn}(\text{L})(\text{H}_2\text{O})]\cdot 5\text{H}_2\text{O}\}_n$ (**1**) and $\{[\text{Cd}(\text{L})(\text{H}_2\text{O})]\cdot \text{H}_2\text{O}\cdot 0.75\text{EtOH}\}_n$ (**2**), derived from dihydrazone ligand with terminal N-donor pyridine moieties were synthesized and characterized. The metal atoms adopt a pentagonal bipyramidal geometry, where the ligand wraps around the metals in the equatorial plane, while their vertexes are occupied by the oxygen atom of water molecule and nitrogen atom of terminal pyridine moiety. This axial coordination of the nitrogen atoms resulted in the formation of 1D coordination polymers in both compounds, as a *zig-zag* like chains, parallel to the crystallographic *b*-axis. The supramolecular architecture of **2** affect the photoluminescent properties. The DFT calculations showed that a decrease in the number of electron states in the top of the valence band may hinder the electron-hole recombination process. The similarity of the electronic structures of coordination polymers **1** and **2** might lead to similarities in their photoluminescence spectra.

Keywords: one-dimensional coordination polymer, X-ray diffraction, Hirshfeld surface, photoluminescence, Density of States.