Synthesis, characterization and crystal structure determination of new coordination polymer of zinc(II) containing N-(4-pyridyl)isonicotinamide ligand

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Abstract: In this study, new coordination polymer was synthesized by the reaction of ZnCl_2 and LNPI carboxamide, (N-(4-pyridyl)isonicotinamide) as well as characterized by FT-IR spectroscopy, elemental analysis (CHN), scanning electron microscope (SEM) and single-crystal X-ray diffraction analysis. The results revealed that the compound [ZnCl_2 (LNPI)]_n as a one-dimensional zig-zag polymeric chain, was crystallized in “orthorhombic” crystalline system with the space group Pca_2. The study of intermolecular interactions and hirshfeld surface analysis showed that the Zn-Cl···H-N hydrogen bond plays an important role in the stability of the polymeric chains in the crystal packing structure. To get more insight about molecular structure and electronic properties of ligand and complex structures, theoretical studies using density functional theory (DFT) method were performed.

Keywords: Coordination polymer; carboxamide; single crystal; hydrogen bond; theoretical study.

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