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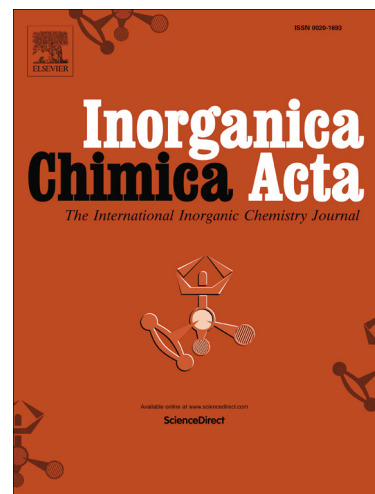
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# Synthesis, spectroscopic characterization, crystal structure, Hirshfeld surface analysis and antimicrobial activities of two triazole Schiff bases and their silver complexes

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## Abstract

The present work describes the synthesis, structural characterization, Hirshfeld analysis, and antibacterial assays of two hydroxy Schiff bases with triazole moiety: *N*-[(*E*)-(3-hydroxy)methylidene]-4*H*-1-2-4 triazol-4-amine (**L1**) and *N*-[(*E*)-(2,4-dihydroxy)methylidene]-4*H*-1-2-4 triazol-4-amine (**L2**). The interaction of these two Schiff bases with AgNO<sub>3</sub> leads to Ag(I) dimer [Ag(**L1**)](NO<sub>3</sub>) in the case of the first ligand (**L1**) and polymer [Ag(**L2**)]<sub>n</sub>(NO<sub>3</sub>)<sub>n</sub>(H<sub>2</sub>O) for (**L2**). Crystal structure determination and Hirshfeld analysis reveal the presence of two important hydrogen bond interactions in the four compounds, O...H and H...N, involving nitrogen atoms of triazole ring. Contribution of these two types of hydrogen bonds evolves inversely from (**L1**) which contains one –OH, to (**L2**) containing two –OH, then to [Ag(**L1**)](NO<sub>3</sub>) dimer and finally to [Ag(**L2**)]<sub>n</sub>(NO<sub>3</sub>)<sub>n</sub>(H<sub>2</sub>O) polymer. Indeed, we observed an increase of the percentage to the Hirshfeld surfaces of O...H contribution from (**L1**) to [Ag(**L2**)]<sub>n</sub>(NO<sub>3</sub>)<sub>n</sub>(H<sub>2</sub>O) passing by (**L2**) and [Ag(**L1**)](NO<sub>3</sub>), while the percentage of N...H decrease in the same way. Antibacterial activity of the free ligands (**L1**), (**L2**) and their silver complexes [Ag(**L1**)](NO<sub>3</sub>) and [Ag(**L2**)]<sub>n</sub>(NO<sub>3</sub>)<sub>n</sub>(H<sub>2</sub>O) were evaluated against four Gram-negative (*E. coli*, *Salmonella typhimurium*, *Klebsiella*

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