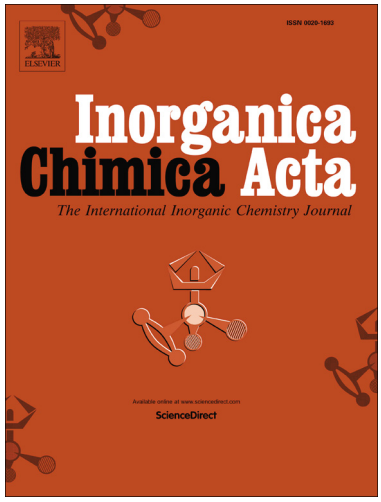

Research paper

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Mixed Phenoxo and Azido Bridged Dinuclear Nickel(II) and Copper(II) Compounds with *N,N,O*-Donor Schiff Bases: Synthesis, Structure, DNA Binding, DFT and molecular docking study

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Abstract

Two dinuclear complexes, μ-phenoxo, $\mu_{1,1}$-azido bridged $[Ni_2(L)_2(\mu_{1,1}\text{-}N_3)(N_3)(CH_3OH)]$ (**1**) and μ-phenoxo, $\mu_{1,1}$-azido bridged $[Cu_2(L)_2(\mu_{1,1}\text{-}N_3)(N_3)]$ (**2**) bearing HL as a blocking co-ligand produced by the 1:1 condensation of N-methyl 1,3 propanediamine with *o*-vanillin have been synthesized and successfully characterized by elemental analyses, IR and electronic spectroscopy, single-crystal X-ray diffraction for **1** and DFT optimization for **2**. X-ray crystal structure discloses that the asymmetric unit of **1** consists of two nickel(II) ions exhibiting a six-coordinate octahedral coordination with μ-phenoxo, $\mu_{1,1}$-azido bridging dimeric structure. The DFT optimization of **2** reveals the five-coordinate distorted square pyramidal geometry around