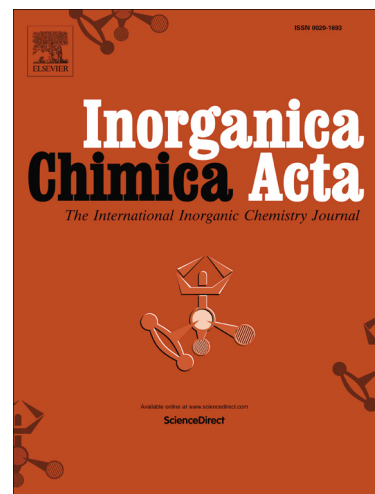


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Research paper

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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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 $[\text{Ni}_2(\text{L})_2(\mu_{1,1}\text{-N}_3)(\text{N}_3)(\text{CH}_3\text{OH})]$ (**1**) and μ -phenoxo, $\mu_{1,1}$ -azido bridged $[\text{Cu}_2(\text{L})_2(\mu_{1,1}\text{-N}_3)(\text{N}_3)]$ (**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

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