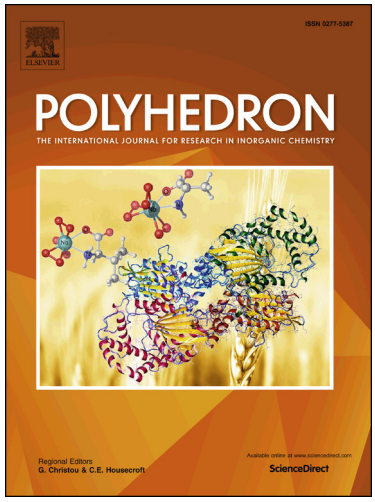

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Synthesis, crystal structure, magnetic properties and DFT study of dinuclear Ni(II) complex with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent

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Abstract

A dinuclear double end-on azido bridged Ni(II) complex $[Ni_2\mathbf{L}_2(\mu\text{-}_{1,1}\text{-}N_3)_2(N_3)_2]$ (**1**) with the condensation product of 2-quinolinecarboxaldehyde and trimethylammonium acetohydrazide chloride (Girard's T reagent) (**HL**Cl) has been synthesized and characterized by elemental analysis, IR spectroscopy, single-crystal X-ray diffraction, magnetic measurements and DFT studies. In complex **1** intra-dimer ferromagnetic coupling between Ni^{2+} ions (J = +12.0(2) cm^{-1}) and inter-dimer antiferromagnetic interaction (δ = –0.8(3) cm^{-1}) were observed. DFT-BS calculations provided explanation of ferromagnetic exchange coupling in complex **1**.

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