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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  $[\text{Ni}_2\text{L}_2(\mu_{-1,1}\text{-N}_3)_2(\text{N}_3)_2]$  (**1**) with the condensation product of 2-quinolinecarboxaldehyde and trimethylammonium acetohydrazide chloride (Girard's T reagent) (**HLCl**) 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  $\text{Ni}^{2+}$  ions ( $J = +12.0(2) \text{ cm}^{-1}$ ) and inter-dimer antiferromagnetic interaction ( $\delta = -0.8(3) \text{ cm}^{-1}$ ) were observed. DFT-BS calculations provided explanation of ferromagnetic exchange coupling in complex **1**.

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