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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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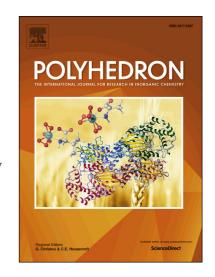
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## **ACCEPTED MANUSCRIPT**

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

Mima Č. Romanović<sup>a</sup>, Božidar R. Čobeljić<sup>a</sup>, Andrej Pevec<sup>b</sup>, Iztok Turel<sup>b</sup>, Vojislav Spasojević<sup>c</sup>, Arshak A. Tsaturyan<sup>d</sup>, Igor N. Shcherbakov<sup>d</sup>, Katarina K. Anđelković<sup>a</sup>, Marina Milenković<sup>e</sup>, Dušanka Radanović<sup>f</sup>, Milica R. Milenković<sup>a1</sup>

#### **Abstract**

A dinuclear double end-on azido bridged Ni(II) complex  $[Ni_2L_2(\mu_{-1,1}-N_3)_2(N_3)_2]$  (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 Ni<sup>2+</sup> ions (J = +12.0(2) cm<sup>-1</sup>) and inter-dimer antiferromagnetic interaction ( $\delta = -0.8(3)$  cm<sup>-1</sup>) were observed. DFT-BS calculations provided explanation of ferromagnetic exchange coupling in complex 1.

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