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Linear hexanuclear nickel complexes with rich electrochemical features and facility to reduction

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Abstract: Two novel linear hexanuclear nickel complexes $[\text{Ni}_6(\mu_6\text{-dpznda})_4\text{Cl}_2](\text{PF}_6)_2$ (**1**) and $[\text{Ni}_6(\mu_6\text{-dpznda})_4(\text{NCS})_2](\text{PF}_6)_2$ (**2**) ($\text{H}_2\text{dpznda} = N^2, N^7$ -di(pyrazin-2-yl)-1,8-naphthyridine-2,7-diamine) were synthesized and structurally characterized. Both the two complexes consist of a linear metal chain and four supporting ligands which are helically wrapped around the metal core. The single crystal X-ray structural analysis showed that the complex **1** belonged to rhombohedral system, space group $R\bar{3}$ with $a = b = 34.2051(8)$, $c = 20.7751(5)$ Å, $V = 21050.2(9)$ Å³ and $Z = 9$. Direct-current magnetic susceptibility measurements showed weak antiferromagnetic interactions with coupling parameters of $g = 2.04$ and $J = -8.27$ cm⁻¹ for **1** and $g = 2.02$ and $J = -12.62$ cm⁻¹ for **2**, respectively ($\hat{H} = -J\hat{S}_1\hat{S}_2$, $S_1 = S_2 = 1$). The decrease of magnetic moments at low temperature was partly attributed to ZFS. The electrochemical study on complex **1** shows rich features and facility to reduction in its cyclic voltammogram by displaying four reversible redox couples at $E_{1/2} = +0.01, -0.29, -0.64$ and -0.73 V (vs. Ag/AgCl).

Keywords: Metal string compounds; Hexanuclear nickel complex; Extended metal atomic chains; Electrochemical features; Magnetic property

1. Introduction

Linear metal string complex, also named as EMACs (extended metal atomic chains), is a kind of polynuclear complexes with metal-metal interaction, which shows unique electromagnetic properties and prospective applications of molecular electronics.[1] Increasing attention has been paid to linear metal string complexes, especially

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