

Experimental and theoretical magnetostructural studies on discrete heterometallic cyanide-bridged dinuclear $\text{Fe}^{\text{III}}\text{Mn}^{\text{II}}$ and tetranuclear $\text{Fe}^{\text{III}}_2\text{Cu}^{\text{II}}_2$ complexes bearing tripodal pyrazolyl borate and tetradentate phenolate-based ligands

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Streszczenie

Two new complexes $[\text{Fe}^{\text{III}}(\text{Tp})(\text{CN})_2(\mu\text{-CN})\text{Mn}^{\text{II}}\text{Cl}(\text{HL}^1)] \cdot 3\text{DMF}$ (**1**) and $\{[\text{Fe}^{\text{III}}(\text{Tp})(\text{CN})(\mu_2\text{-NC})_2\text{Cu}^{\text{II}}(\text{HL}^2)](\text{ClO}_4)\}_2 \cdot 6\text{DMF}$ (**2**) ($\text{HL}^1 = 2\text{-}(((1\text{-methylbenzimidazol-2-yl)methyl})(\text{pyridin-2-ylmethyl})\text{amino})\text{methyl})\text{phenol}$ and $\text{HL}^2 = 2\text{-}(((\text{pyridin-2-ylmethyl})(\text{quinolin-2-ylmethyl})\text{-amino})\text{methyl})\text{phenol}$) have been synthesized and characterized by elemental analysis and IR and UV/vis spectroscopy. Structural analysis revealed that **1** is a discrete dinuclear coordination complex and **2** is a discrete tetranuclear coordination complex. In complex **1**, each Mn^{II} is in a distorted octahedral MN_4OCl environment where coordination is satisfied by three nitrogen atoms and one oxygen atom of the ligand, and a chloride group and one nitrogen atom from cyanide. In complex **2**, each Cu is in a distorted octahedral MN_5O environment where coordination is satisfied by three nitrogen atoms and one oxygen atom of the ligand, and two nitrogen atoms from two cyanides. Direct current (dc) variable-temperature magnetic susceptibility measurements on polycrystalline samples of **1** and **2** were carried out in the temperature range of 1.8–300 K. Investigation of the magnetic properties reveals the occurrence of weak antiferromagnetic coupling between the low-spin Fe^{III} ($S = 1/2$) ions and high-spin Mn^{II} ($S = 5/2$) ions in **1**, while **2** exhibits ferro- and antiferromagnetic coupling between the metal ions in the tetranuclear $\text{Cu}^{\text{II}}_2\text{Fe}^{\text{III}}_2$ unit. DFT calculations show ferromagnetic coupling in both complexes, although this appears to be weak in the case of complex **1**. In addition, magnetostructural correlations reveal the magnetic behavior against Mn–N–C and Fe–C–N angles in **1** and Cu–N–C and Fe–C–N angles in **2**.

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