Magnetic properties and molecular structure of a binuclear alternative bridged Cu(II)Re(IV) complex containing a macrocyclic ligand.

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Two novel macrocyclic compounds, the heterobimetallic complex $\{(CuL_\alpha)[ReCl_4(ox)]\}_n$ (**1**) and the mononuclear complex $[CuL_\alpha]\cdot 2ClO_4$ (**2**) (where L_α = *N-meso*-5,12-Me_2-7,14-Et_2-[14]-4,11-dieneN_4), have been synthesized and their crystal structures were determined by the single-crystal X-ray diffraction technique. Complex **1** crystallizes in the monoclinic space group $P2_1/c$, whereas **2** crystallizes in the monoclinic space group $P2_1/n$. The $[CuL_\alpha]^{2+}$ macrocyclic cation in **1** is coordinated from above and below by $[ReCl_4(ox)]^{2-}$ units through the chloro- and monodentate oxalato ligands, and this creates an alternating chloro-oxalato-bridged heterometallic Re^{IV}–Cu^{II} one-dimensional zig-zag chain. Their magnetic measurements were carried out over the temperature range 1.8–300 K using a Quantum Design SQUID magnetometer (MPMSxL-5 type). Compound **1** behaves like a ferrimagnetic Cu^{II}–Re^{IV} dimetallic chain with two intrachain antiferromagnetic coupling parameters and strong single-ion anisotropy, D(Re) = 109 cm^{-1}. Compound **2** shows weakly interacting paramagnetic centers in the crystal lattice. The effects of hydrogen bonds mediating the magnetic exchange interactions on the spin density have been evidenced by DFT calculations.

Słowa kluczowe

building block, bimetallic complexes, alternating chain, Exchange interaction, ferrimagnetic properties

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