

Synthesis, crystal structure and magnetic properties of new molecular, macrocyclic building blocks of Ni(II) and Cu(II).

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Streszczenie

New macrocyclic building blocks $[\text{NiL}_1\text{Cl}_2]$ (**1**) ($\text{L}_1 = \text{N-dl-2,9-dimethyl-1,5,8,12-tetraazacyclotetradecan}$) and $[\text{CuL}_2(\text{ClO}_4)_2]$ (**2**) ($\text{L}_2 = \text{N-d-2,3,9,10-tetramethyl-1,5,8,12-tetraazacyclotetradeka-1,8 diene}$) were synthesized and the crystal structure of both compounds were determined. Complexes **1** and **2** crystallizes in monoclinic, space group P 21/c. Their magnetic properties were studied over the temperature range 1.8–300 K using a Quantum Design SQUID magnetometer (MPMSXL-5-type). The results indicate that both compounds behave as weakly interacting paramagnetic centers in the crystal lattice. The effects of hydrogen bond mediating the magnetic exchange interactions on the spin density have been evidenced by DFT calculations.

Słowa kluczowe

copper (II) and nickel(II) complexes, macrocyclic ligands, building block, magnetic behavior

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