A new molecular building blocks : synthesis, crystal structure, magnetic and spectroscopic properties of Cu(II) and Ni(II) macrocyclic complexes.

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Streszczenie

New higly unsaturated macrocyclic building blocks [CuLSCN]·ClO_4 (**1**) (L = *N-dl*-5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene) and [NiL$(SCN)_2$] (**2**) (L = *N-dl*-5,12-dimethyl-7,14-diisopropyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene) were synthesized and the crystal structures of both compounds were determined. Both complexes crystallizes in monoclinic, space group $P2_1/n$ (**1**) and $P2_1/c$ (**2**). 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. The NIR–Vis–UV diffuse-reflectance electronic spectra confirm the square pyramidal and octahedral geometry around Cu^{2+} and Ni^{2+} metal ions.

Słowa kluczowe

building block, Pentacoordinate Cu(II) complex, macrocyclic complexes, Exchange interactions

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