# Magnetic properties and DMRG modeling of the 1D bimetallic thiocyanate bridged compound {($CuL_1$)[$Co(NCS)_4$]} ($L_1$ =*N*-rac-5,12-$Me_2$-[14]-4,11-dien$eN_4$).

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The magnetic properties of the bimetallic compound {($CuL_1$)[$Co(NCS)_4$]}, where $L_1$ = *N*-rac-5,12-dimethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene have been numerically analysed on the basis of the anisotropic Heisenberg spin-chain model. In the model the single-ion anisotropy of the Co(II) ions is taken into account and the interchain interactions are neglected. The thermodynamic properties are calculated using the DMRG technique adapted to the molecular-based chains for the first time which is reliable in the entire temperature region. The high accuracy results of our simulations have been successfully fitted to the corresponding experimental susceptibility and magnetization data measured for the powder sample and the model parameters (the exchange coupling *J*, the absolute value of the anisotropy constant *D*, the anisotropic *g* factors) have been estimated. The quantum model parameters are consistent with the previous findings, although the ferromagnetic interactions between Cu(II) and Co(II) ions through the thiocyanate bridge are somewhat weaker ($J/k_B$ = 1.0 ± 0.1) than found before.

Słowa kluczowe

Crystal structure, Heterobimetallic chain, Thiocyanate bridge, Magnetism, DMRG technique, Anisotropy constant D of Co(II) ion

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