

Anisotropy and magnetic properties of the bimetallic thiocyanate-bridged chains: density-matrix renormalization approach.

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Streszczenie

Magnetic properties of bimetallic thiocyanate-bridged chains are numerically analyzed on the basis of the one-dimensional quantum anisotropic Heisenberg model without the mean-field corrections. The single-ion and g factor anisotropy of the metal ions (Co(II), Mn(II), Ni(II)) are taken into account. The thermodynamic properties are calculated using the DMRG technique, which is reliable in the entire temperature region, adapted to the molecular-based chains. The high accuracy results of our simulations are successfully fitted to the corresponding experimental susceptibility and magnetization data measured for a powder sample. Our analysis permitted determination of the microscopic parameters (the strength of magnetic couplings between the copper and metal ions and the single-ion anisotropy terms) as well as the corresponding g factors which are consistent with the values known for other compounds.

Słowa kluczowe

crystal structure, Heterobimetallic chain, Thiocyanate bridge, magnetism, DMRG technique, Single-ion anisotropy of Co(II), Mn(II), Ni(II) ions

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