Generalized Heisenberg-Type Magnetic Phenomena in Nickel-Lanthanide Dinuclear Units Assembled in Coordination Polymers by Dicyanomide Ligands

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A new family of $3d$-$4f$ coordination polymers containing the dimeric units Ni^{2+}-Ln^{3+}, where the lanthanides Ln = Eu (**1**), Gd (**2**), Tb (**3**), Dy (**4**), Ho (**5**), has been synthesized in a current search for new single-molecule magnet (SMM) materials [1]. Its magnetic properties have been established by DC and AC magnetometry and explained quantitatively by comprehensive phenomenological modelling. Single-crystal X-ray diffraction study has shown that the lanthanide atoms occupy a nine-coordination site with Muffin-like geometry and individual Ni^{II}-Ln^{III} units are linked by dicyanamide anions. Beside paramagnetic compound **1**, **2-5** exhibit intra-unit ferromagnetic $3d$-$4f$ interactions favourable for a large spin ground state. Due to the easy-plane anisotropy driven energy structure that is unpropitious for the SMM behaviour, a slow field-induced relaxation of magnetization has been observed only in compound **4**. However, a substantial energy barrier U_{eff}/k_B = 26.2 K against spin reversal has been established below 6 K and experimental support for the scenario of the relaxation phenomenon in systems with the Kramers ground state doublet and hyper-fine interactions has been provided. The materials studied provide excellent test-beds for validation of generalized Heisenberg-type model as a tool to simulate the $3d$-$4f$ complexes that was hypothesized in a pioneering DFT approach [2].

References:

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