New tetranuclear manganese clusters with $[Mn_3^{II}Mn^{III}]$ and $[Mn_2^{II}Mn_2^{III}]$ metallic cores exhibiting low and high spin ground state.

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Streszczenie

Two tetranuclear mixed-valent clusters, $[Mn^{II}_3Mn^{III}Cl(Ph_3CCOO)_4(CH_3OCH_2CH_2O)_4(CH_3CN)]\cdot 0.4C_6H_5CH_3\cdot 0.6CH$ (**1**) with an unprecedented $[Mn^{II}_3Mn^{III}]$ core and $[Mn^{II}_2Mn^{III}_2Cl_4(CH_3OCH_2CH_2O)_6]$ (**2**), were synthesized and characterized by single-crystal X-ray diffraction and magnetic measurements. Their properties were analyzed in the framework of phenomenological modelling and DFT calculations, showing acceptable agreement between theory and experiment. Both building blocks $[Mn^{II}_3Mn^{III}]$ and $[Mn^{II}_2Mn^{III}_2]$ provide good examples of bipartite systems with the lowest S_T = 1/2 and highest S_T = 9 magnetic ground states available for them. The topology of the magnetic interactions in the $[Mn^{II}_3Mn^{III}]$ core provides a suitable template for the molecular qubit implementation and the stability of the spin-1/2 ground state strongly depends on the antiferromagnetic Mn^{II}–Mn^{II} coupling.

Adres publiczny

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