Tetranuclear manganese complexes with $[Mn^{II}_4]$ and $[Mn^{II}_2Mn^{III}_2]$ units: syntheses, structures, magnetic properties, and DFT study.

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Abstract

Two tetranuclear manganese compounds, $[Mn_4(\mu_3,\eta^2\text{-}L)_4Br_4(LH)_4]$ (**1**) and $[Mn_4(\mu_3,\eta^2\text{-}L)_2(\mu,\eta^2\text{-}L)_4L_2Br_2]$ (**2**), with cubane and defect dicubane-like cores were synthesized and characterized by single-crystal X-ray diffraction, magnetic measurements, and DFT calculations (LH = 2-methoxyethanol). The magnetic properties of the resulting $[Mn_4]$ building blocks are presented and discussed in detail. In particular, in **2** the Mn^{III}–O–Mn^{III} angle 103.12(8)° is the largest observed to date for such a system. The conjunction of antiferromagnetic and ferromagnetic interactions within the tetranuclear mixed-valent $Mn^{II}_2Mn^{III}_2$ complexes results in an unusual S_T = 1 ground state.

Słowa kluczowe

manganese, metal alcoxides, synthetic methods, X-ray diffraction, magnetic properties

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