Family of $Mn_4^{III}Ln_2^{III}$ (Ln^{III} = Sm^{III}, Gd^{III}, Dy^{III}) coordination clusters : experimental and theoretical investigations.

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Streszczenie

The present work introduces a family of $Mn^{III}_4Ln^{III}_2$ (Ln^{III} = Sm^{III}, Gd^{III}, Dy^{III}) coordination clusters having a multisite hydroxyl rich ligand, 3-[(2-hydroxy-3-methoxy-benzylidene)-amino]-propane-1,2-diol (H_3Vapd), namely $[Mn^{III}_4Sm^{III}_2(Vapd)_4(OAc)_6]\cdot 4H_2O$ (**1**), $[Mn^{III}_4Gd^{III}_2(Vapd)_4(OAc)_6]\cdot 4H_2O$ (**2**) and $[Mn^{III}_4Dy^{III}_2(Vapd)_4(OAc)_6]\cdot 4H_2O$ (**3**). The Sm^{III} analog is the first example of a Mn_4Ln_2 species reported to date. The similarities and differences in terms of structure, topology and magnetic behaviors within the series are investigated extensively. DFT computations were carried out for $Mn^{III}_4Gd^{III}_2$ to address the experimentally challenging questions regarding the nature of the magnetic interactions in this cluster.

Słowa kluczowe

manganese, lanthanides, density functional calculations, magnetic properties

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