



Effect of diamagnetic Zn(II) ions on the SMM properties of a series of trinuclear ZnDy₂ and tetranuclear Zn₂Dy₂ (Ln^{III} = Dy, Tb, Gd) complexes: combined experimental and theoretical studies

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Streszczenie

To study the effect of diamagnetic ions on magnetic interactions, utilizing a compartmental ligand (Z)-2-(hydroxymethyl)-4-methyl-6-((quinolin-8-ylimino)methyl)phenol (LH₂), two different series of Zn^{II}–Ln^{III} complexes, namely the trinuclear series of [DyZn₂(L)₂(μ₂-OAc)₂(CH₃OH)₂]·NO₃·MeOH (**1**), [TbZn₂(L)₂(μ₂-OAc)₂(CH₃OH)₂]·NO₃·5MeOH·H₂O (**2**), and [GdZn₂(L)₂(μ₂-OAc)₂(CH₃OH)₂]·NO₃·MeOH·CHCl₃ (**3**) and the tetranuclear series of [Dy₂Zn₂(LH)₄(NO₃)₄(μ₂-OAc)]·NO₃·MeOH·H₂O (**4**), [Tb₂Zn₂(LH)₄(NO₃)₄(μ₂-OAc)]·NO₃·MeOH·2H₂O (**5**), and [Gd₂Zn₂(LH)₄(NO₃)₄(μ₂-OAc)]·NO₃·MeOH·2H₂O (**6**), were synthesized. Trinuclear Zn^{II}–Ln^{III} complexes **1–3** consist of one Ln^{III} ion sandwiched between two peripheral Zn^{II} ions forming a bent type Zn^{II}–Dy^{III}–Zn^{II} array with an angle of 110.64°. Tetranuclear Zn^{II}–Ln^{III} complexes **4–6** are basically a combination of two dinuclear moieties of [LnZn(LH)₂(NO₃)₂]⁺ connected by one bidentate bridging acetate ion in μ₂-OAc coordination mode. The detailed magnetic analysis reveals that complexes **1** and **4** are single molecule magnets having energy barriers of 34.98 K and 46.71 K with relaxation times (τ₀) of 5.05 × 10^{−4} s and 5.24 × 10^{−4} s, respectively. *Ab initio* calculations were employed to analyze the magnetic anisotropy and magnetic exchange interaction between the Zn^{II} and Ln^{III} centers with the aim of gaining better insights into the magnetic dynamics of complexes **1–6**.

Adres publiczny

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