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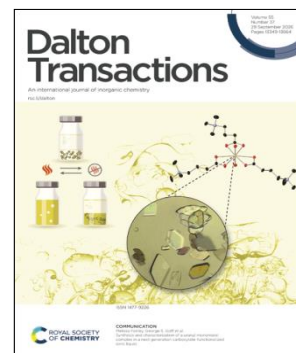
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Title: Magneto-structural correlations in multinuclear Dy/Zn complexes: controlling magnetic relaxation through anisotropy and exchange interactions

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Abstract: The rational design of lanthanide-based single-molecule magnets (SMMs) requires an understanding of how structural variations influence magnetic anisotropy, exchange interactions, and relaxation dynamics. Herein, we report a family of multinuclear Dy(iii)/Zn(ii) complexes supported by a compartmental Schiff-base ligand, including two tetranuclear Dy₄ clusters, [Dy₄(L)₂(HL)₂(μ-OH)₂(NO₃)₂](NO₃)₂·H₂O (1) and [Dy₄(L)₂(μ-OH)₂(μ-pnba)₄(pnba)₂](NO₃)₂·3CH₃CN (2), and two heterometallic Zn-containing complexes, [Zn₂Dy₂(L)₂(μ-CO₃)₂(NO₃)₂](NO₃)₂·0.5H₂O·CH₃OH (3) and [ZnDy(L)(μ-tfa)(hfac)]₂ (4). Single-crystal X-ray diffraction studies reveal that variations in the bridging modes, coordination environments, and metal-ion arrangements generate distinct structural motifs. Magnetic studies demonstrate diverse magnetic behaviours arising from differences in Dy(iii) magnetic interactions and relaxation pathways. In particular, the Dy₄ complexes exhibit different magnetic responses despite comparable Dy···Dy separations, indicating that the relative arrangement of the Dy(iii) coordination environments plays a crucial role in determining the nature of magnetic interactions. Ab initio CASSCF calculations provide further insight into the relationship between structural features and magnetic properties by revealing variations in Dy(iii) magnetic anisotropy and easy-axis orientations. The Zn-containing complexes further highlight the influence of magnetic-ion arrangement and nuclearity on relaxation dynamics. Correlation of structural, magnetic, and theoretical results suggests that the orientation of Dy(iii) anisotropy axes, together with the balance between exchange and dipolar interactions, governs the observed magnetic behaviour. This study provides insights into the magneto-structural relationships controlling magnetic relaxation in multinuclear Dy-based complexes.



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