ELECTRONIC SUPPLEMENTARY INFORMATION

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A family of dinuclear lanthanide(III) complexes from the use of a tridentate Schiff base: structural and physical studies, and the case of a Dy^{III}_2 emissive single-molecule magnet†

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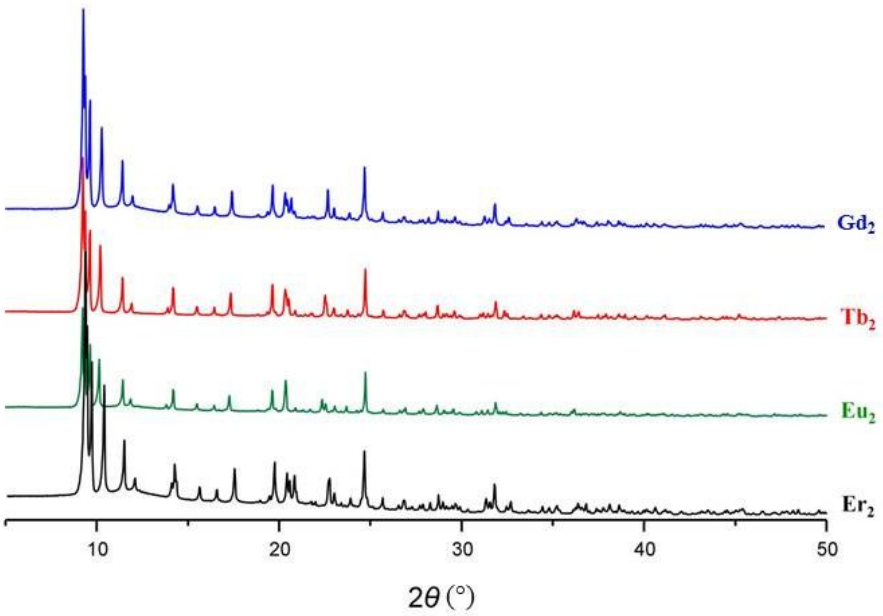

Fig. S1 Powder XRD diagrams' comparison between the representative Eu^{III}_2 (**2**), Gd^{III}_2 (**3**), Tb^{III}_2 (**4**) and Er^{III}_2 (**7**) complexes. The experimental pattern of the Gd^{III}_2 complex **3** shown above is identical with the theoretical diagram for this complex and for the Dy^{III}_2 complex **5** (the structures of **3** and **5** were solved by single-crystal, X-ray crystallography).

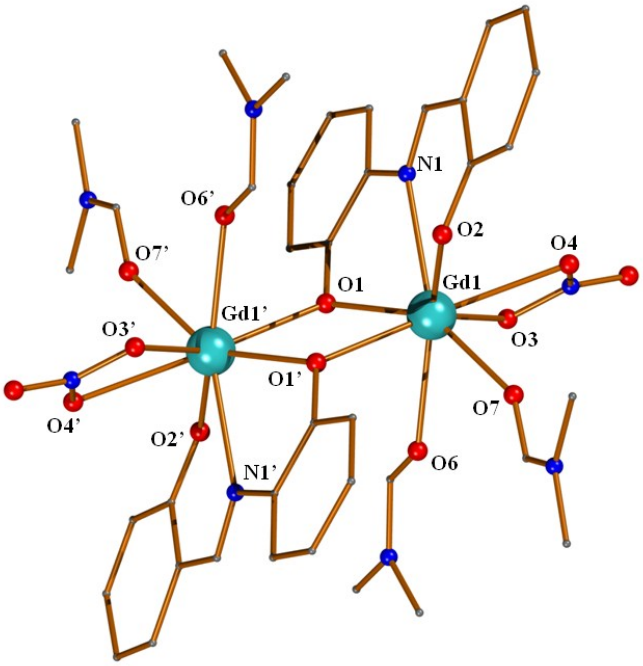

Fig. S2 Partially labelled plot of the molecular structure of complex $[Gd_2(NO_3)_2(saph)_2(DMF)_4]$ (**3**). Unprimed and primed atoms are related by the symmetry operation $-x+2, -y, -z$.

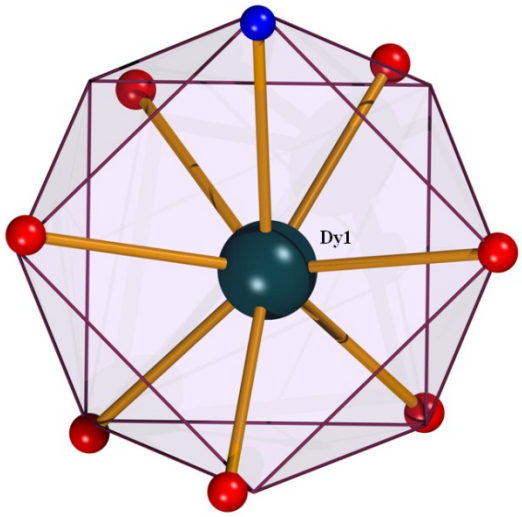

Fig. S3 Another view (different than the one shown in Fig. 2 of the main text) of the coordination polyhedron of Dy1 in the structure of **5**. Colour scheme: Dy1, dark green; N, blue; O, red.

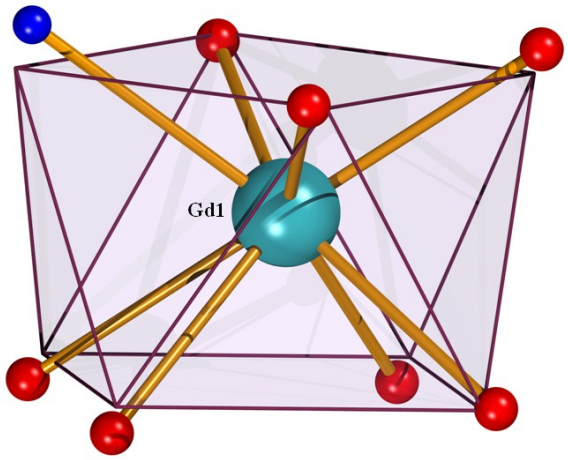

Fig. S4 The square antiprismatic coordination geometry of Gd1 in the structure of **3**. The plotted polyhedron is the ideal, best-fit polyhedron using the program SHAPE. Colour scheme: Gd1, sky blue; N, blue; O, red.

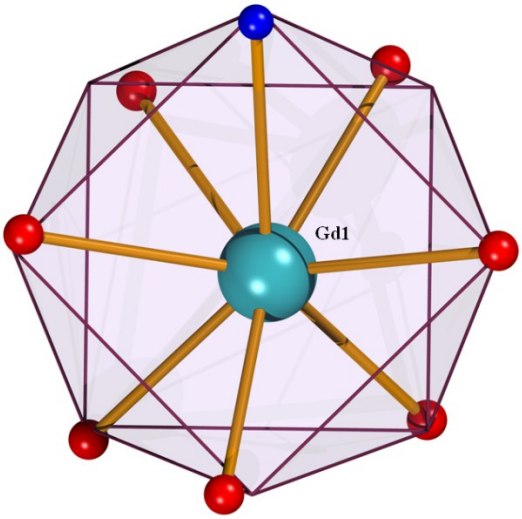

Fig. S5 Another view (different than the one shown in Fig. S4) of the coordination polyhedron of Gd1 in the structure of **3**. Colour scheme: Gd1, sky blue; N, blue; O, red.

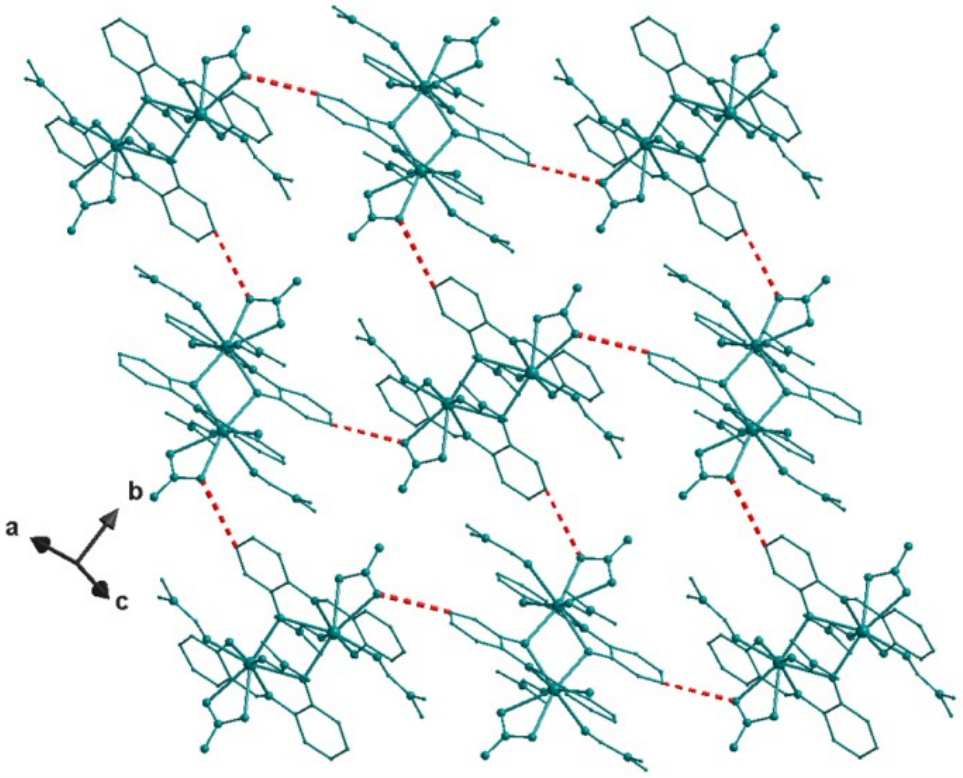

Fig. S6 A small portion of one 2D layer in the crystal structure of complex **3**, resulting from the intermolecular C3-H3···O4 (and symmetry equivalent) hydrogen bonding interaction.

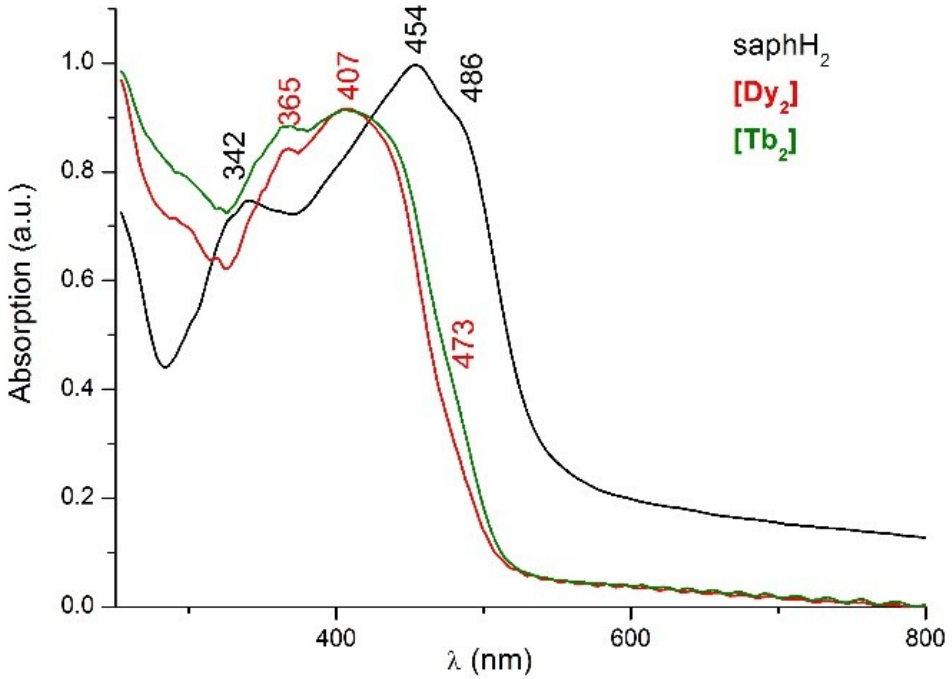

Fig. S7 Solid-state UV-VIS absorption spectra of free H_2saph and complexes **4** and **5**.

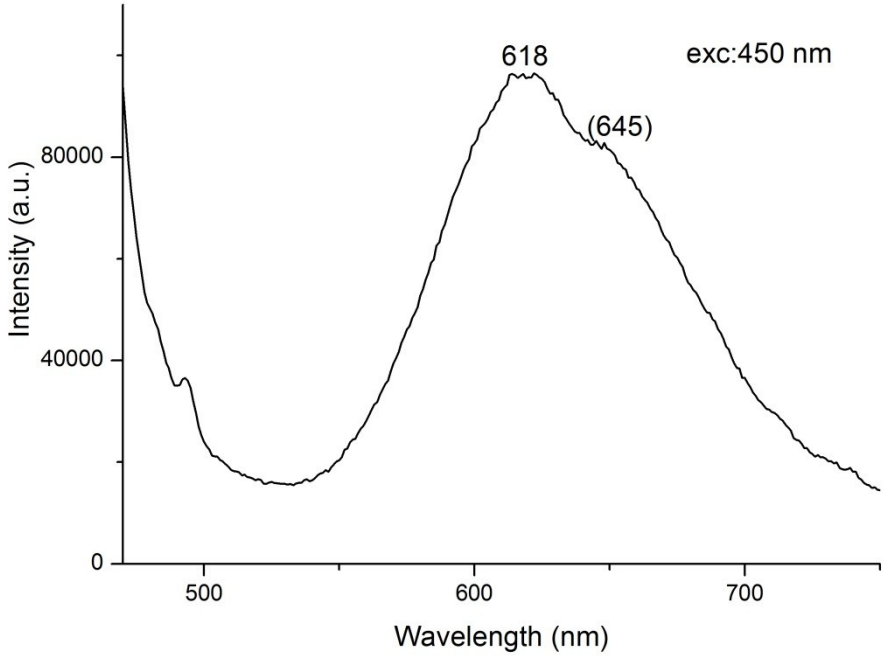

Fig. S8 Solid-state, room-temperature emission spectrum of the free ligand H_2saph upon maximum excitation at 450 nm.

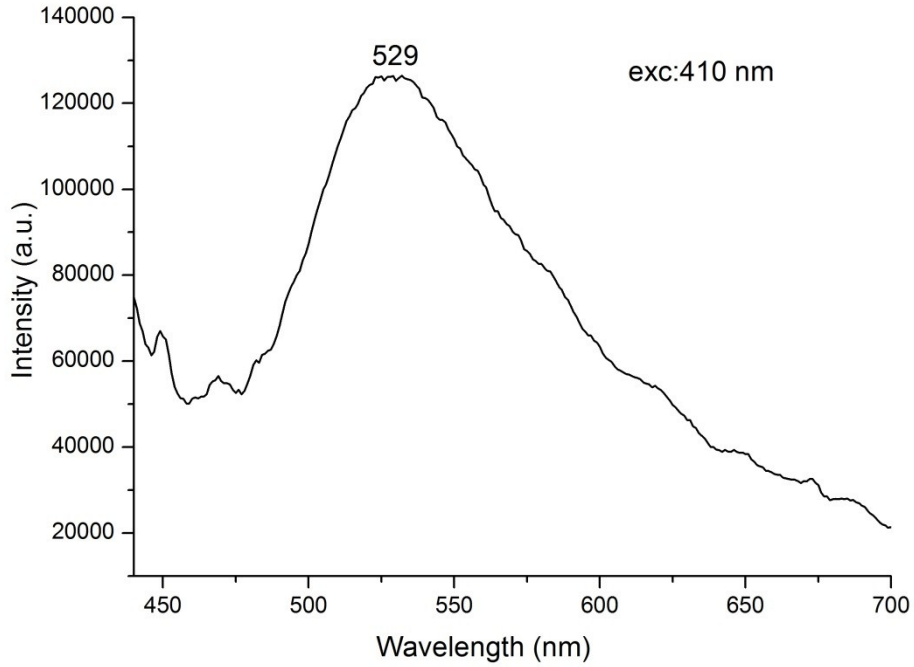

Fig. S9 Solid-state, room-temperature emission spectrum for the Sm^{III}_2 complex **1**; the excitation wavelength was 410 nm.

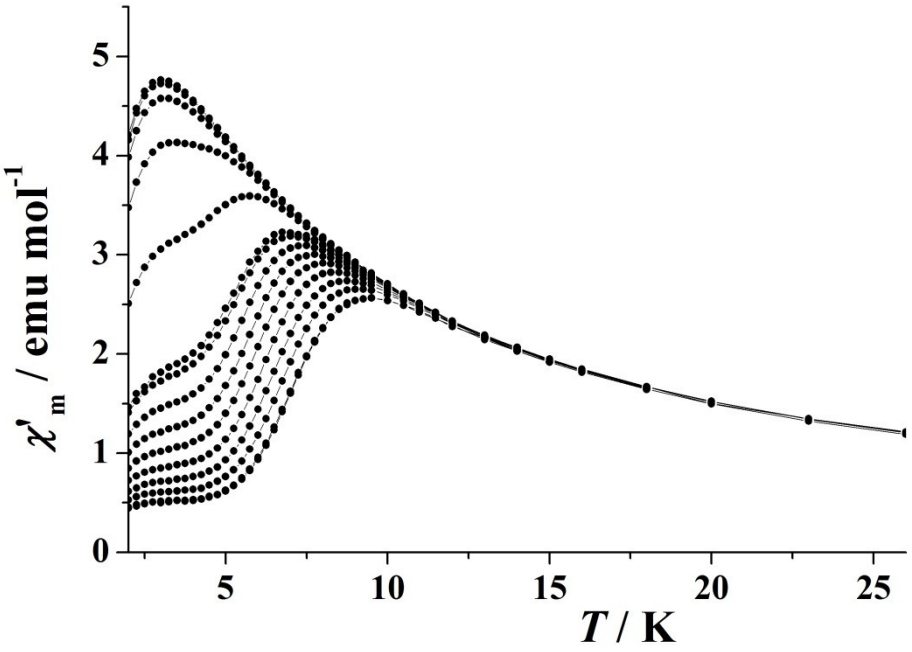

Fig. S10 Temperature dependence of the in-phase (χ_M') component of the ac susceptibility for **5** under a zero external dc field at various frequencies.

Table S1. Important crystallographic data for complexes $[Gd_2(NO_3)_2(saph)_2(DMF)_4]$ (**3**) and $[Dy_2(NO_3)_2(saph)_2(DMF)_4]$ (**5**).

	Complex **3**	Complex **5**
Formula	$C_{38}H_{46}Gd_2N_8O_{14}$	$C_{38}H_{46}Dy_2N_8O_{14}$
Fw	1153.33	1163.83
Space group	$P2_1/n$	$P2_1/n$
a (Å)	12.3327(2)	12.3132(2)
b (Å)	14.0747(3)	14.0547(2)
c (Å)	12.6772(2)	12.6042(2)
α (º)	90.00	90.00
β (º)	91.259(1)	91.412(1)
γ (º)	90.00	90.00
V (Å^3)	2199.97(7)	2180.60(6)
Z	2	2
T (ºC)	-113	-113
Radiation	Cu Kα (1.54178 Å)	Cu Kα (1.54178 Å)
ρ_{calcd} (g cm^{-3})	1.741	1.773
μ (mm^{-1})	19.917	18.755
Reflections with $I>2\sigma(I)$	3444	3516
$R_1[I>2\sigma(I)]$[a]	0.0355	0.0364
$wR_2[I>2\sigma(I)]$[a]	0.0892	0.0973

[a] $w=1/[\sigma^2(F_o^2)+(aP)^2+bP]$ and $P = [\max(F_o^2,0)+2F_c^2]/3$,
$R_1 = \Sigma(|F_o|-|F_c|)/\Sigma(|F_o|)$ and $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Table S2. Continuous Shape Measures (CShM) values for the possible coordination polyhedra of the 8-coordinate Gd1/Gd1' and Dy1/Dy1' ions in the molecular structures of the centrosymmetric complexes **3** and **5**, respectively.[a,b]

Ideal polyhedron	Gd1/Gd1' (complex **3**)	Dy1/Dy1' (complex **5**)
Octagon	33.06374	32.95967
Heptagonal pyramid	21.27010	21.45814
Hexagonal bipyramid	16.00208	16.02660
Cube	9.21212	9.17978
Square antiprism	**1.68114**	**1.63634**
Triangular dodecahedron	1.92532	1.82971
Johnson gyrobifastigium	16.85700	16.81023
Johnson elongated triangular bipyramid	26.65569	26.72859
Biaugmented trigonal prism J50	3.38231	3.27316
Biaugmented trigonal prism	2.77170	2.66138
Snub diphenoid	5.36155	5.26433
Triakis tetrahedron	9.96685	9.92229
Elongated trigonal bipyramid	23.10065	23.18327

[a]The smallest values (in bold) define the best polyhedron (square antiprism for **3** and **5**). [b]Chemically significant distortions give CShM values of 0.1 or higher, while values larger than about 3 indicate important distortions.