Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A series of heterospin complexes based on lanthanides and pyridine biradicals: synthesis, structure and magnetic properties

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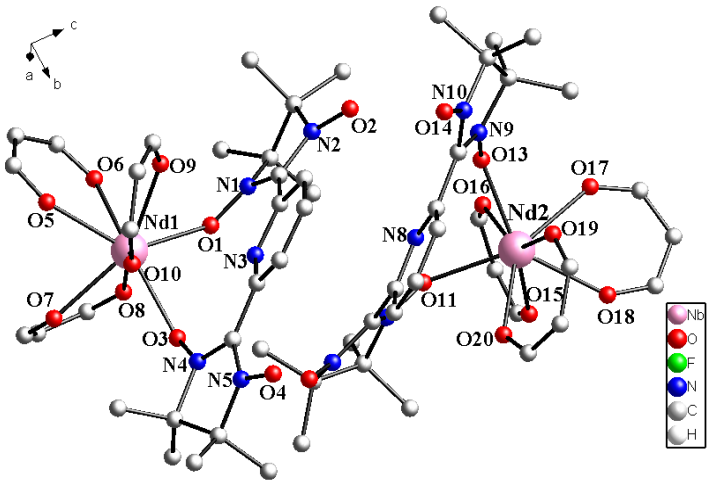


Fig. S1 Simplified view of the crystal structure of **2**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

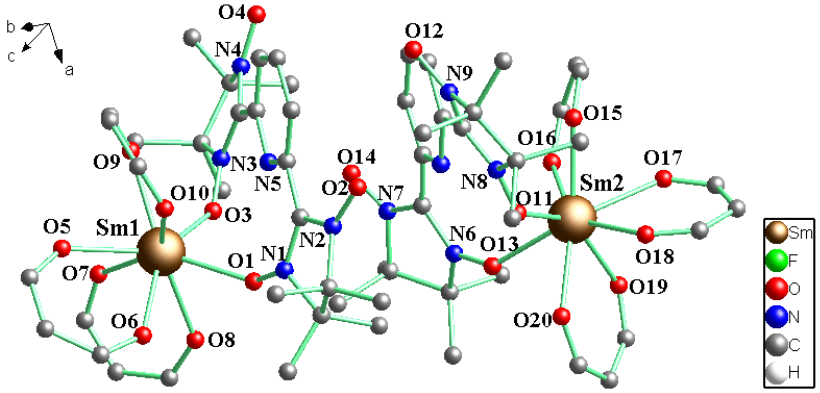


Fig. S2 Simplified view of the crystal structure of **3**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

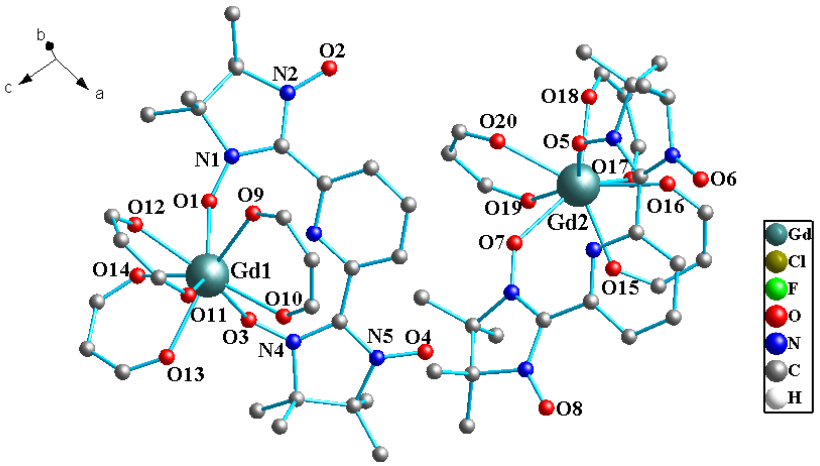


Fig. S3 Simplified view of the crystal structure of **4**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

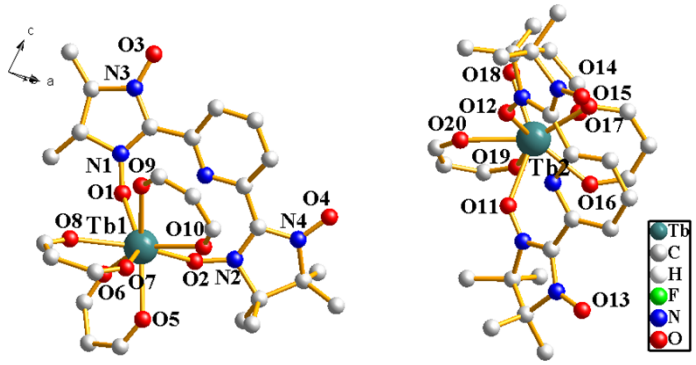


Fig. S4 Simplified view of the crystal structure of **5**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

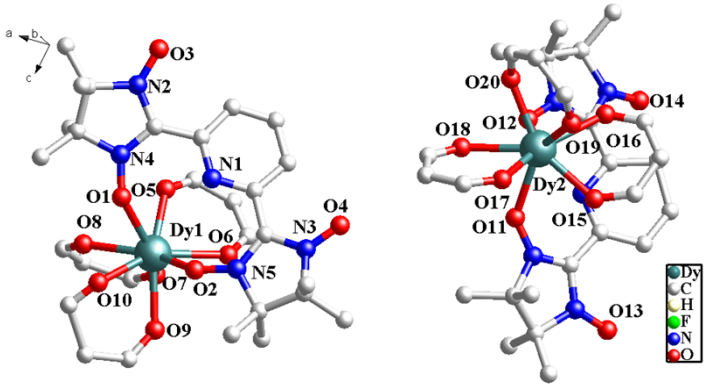


Fig. S5 Simplified view of the crystal structure of **6**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

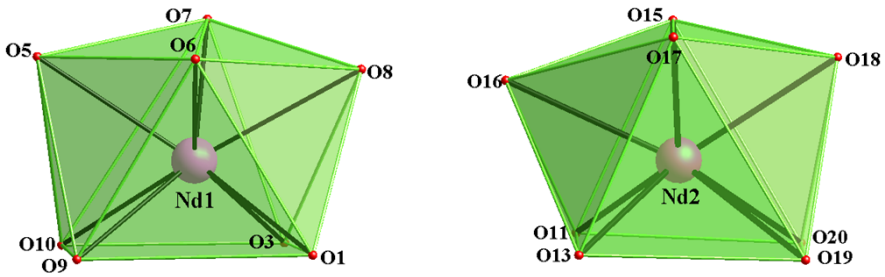


Fig. S6 The coordination polyhedral of Nd(III) in complex **2**.

Table S1. δ (°) and φ (°) values for complex **2**.

	Nd1		Nd2		DD	TP	SAP
δ_1	O10 [O9 O3] O1^a	1.3	O11 [O13 O20] O19^a	0.5	29.5	0.0	0.0
δ_2	O5 [O7 O6] O8^a	16.6	O16 [O15 O17] O18^a	27.1	29.5	21.8	0.0
δ_3	O5 [O9 O6] O1^a	47.6	O16[O13 O17] O19^a	53.3	29.5	48.2	52.4
δ_4	O10 [O7O3] O8^a	55.6	O11 [O15 O20] O18^a	41.8	29.5	48.2	52.4
φ_1	O6–O3–O5–O10^b	24.3	O17–O20–O16–O11^b	9.1	0.0	14.1	24.5
φ_2	O7–O9–O8–O1^b	17.1	O15–O13–O18–O19^b	22.9	0.0	14.1	24.5

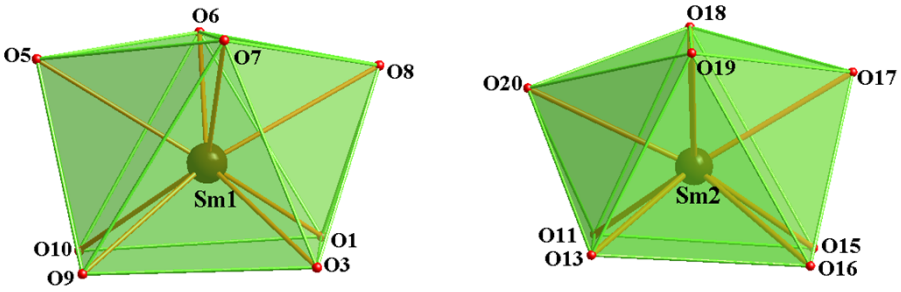


Fig. S7 The coordination polyhedral of Sm(III) in complex **3**.

Table S2. δ (°) and φ (°) values for complex **3**.

	Sm1		Sm2		DD	TP	SAP
δ_1	O10 [O9 O1] O3[a]	1.2	O11 [O13 O15] O16[a]	0.2	29.5	0.0	0.0
δ_2	O5 [O6 O7] O8[a]	17.3	O20 [O18 O19] O17[a]	27.9	29.5	21.8	0.0
δ_3	O5 [O9 O7] O3[a]	41.1	O20 [O13 O19] O16[a]	51.8	29.5	48.2	52.4
δ_4	O10 [O6 O1] O8[a]	50.2	O11 [O18 O15] O17[a]	40.3	29.5	48.2	52.4
φ_1	O7–O1–O5–O10[b]	22.0	O19–O15–O20–O11[b]	8.2	0.0	14.1	24.5
φ_2	O6–O9–O8–O3[b]	12.5	O18–O13–O17–O16[b]	20.9	0.0	14.1	24.5

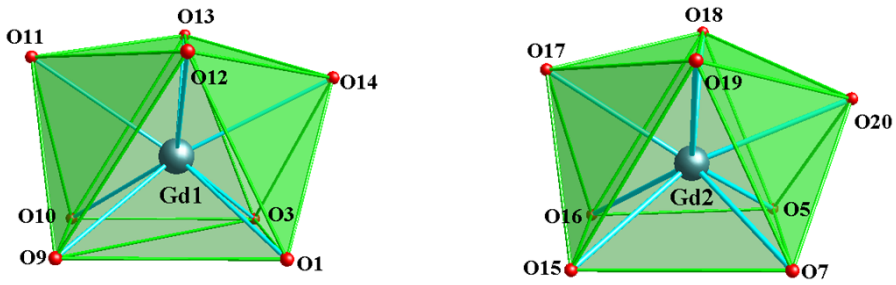


Fig. S8 The coordination polyhedral of Gd(III) in complex **4**.

Table S3. δ (°) and φ (°) values for complex **4**.

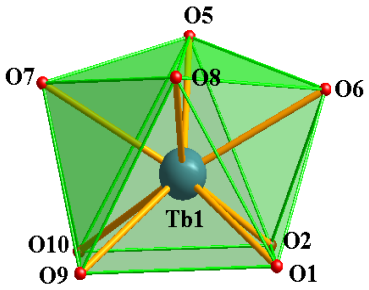
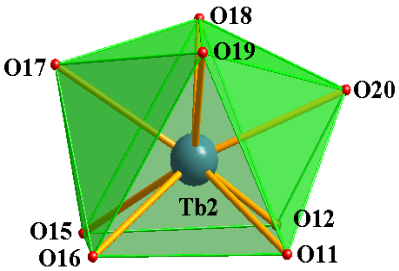
		Gd2			SAP
δ_1		O16 [O15 O5]			0.0
δ_2		O17 [O18 O19			0.0
δ_3		O17 [O15O19			52.4
δ_4		O16[O18 O5]			52.4
φ_1		O19–O5–O17-			24.5
φ_2		O18–O15–O2(			24.5

Fig. S9 The coordination polyhedral of Tb(III) in complex **5**.

Table S4. δ (°) and φ (°) values for complex **5.**

	Tb1		**Tb2**		DD	TP	SAP
δ_1	O10 [O9 O2] O1[a]	1.3	O15 [O16 O12] O11[a]	0.5	29.5	0.0	0.0
δ_2	O7 [O5 O8] O6[a]	21.1	O17 [O18 O19] O20[a]	29.2	29.5	21.8	0.0
δ_3	O7 [O9 O8] O1[a]	47.3	O17 [O16 O19] O11[a]	41.4	29.5	48.2	52.4
δ_4	O10 [O5 O2] O6[a]	53.4	O15[O18 O12] O20[a]	51.7	29.5	48.2	52.4
φ_1	O8–O2–O7–O10[b]	23.6	O19–O12–O17–O15[b]	21.5	0.0	14.1	24.5
φ_2	O5–O9–O6–O1[b]	15.4	O18–O16–O20–O11[b]	7.9	0.0	14.1	24.5

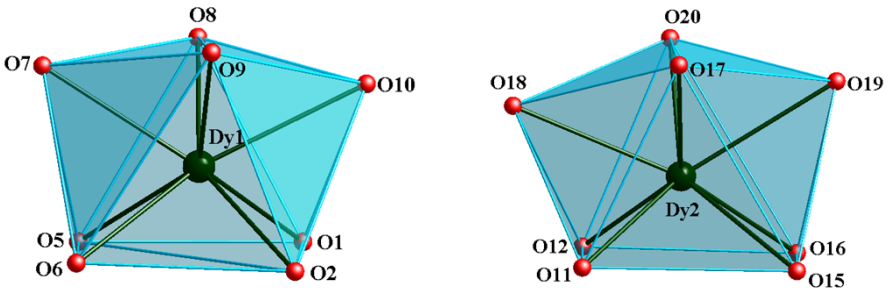


Fig. S10 The coordination polyhedral of Dy(III) in complex **6**.

Table S5. δ (°) and φ (°) values for complex **6**

	Dy1		**Dy2**		DD	TP	SAP
δ_1	O5 [O6 O1] O2[a]	1.886	O12 [O11 O16] O15[a]	0.0793	29.5	0.0	0.0
δ_2	O7 [O8 O9] O10[a]	20.848	O18 [O20 O17] O19[a]	29.244	29.5	21.8	0.0
δ_3	O7 [O6 O9] O2[a]	40.649	O18 [O11 O17] O15[a]	50.778	29.5	48.2	52.4
δ_4	O5 [O8 O1] O10[a]	48.670	O12 [O20 O16] O19[a]	40.056	29.5	48.2	52.4
φ_1	O9–O1–O7–O5[b]	19.350	O17–O16–O18–O12[b]	8.453	0.0	14.1	24.5
φ_2	O8–O6–O10–O2[b]	12.465	O20–O11–O19–O15[b]	19.46	0.0	14.1	24.5

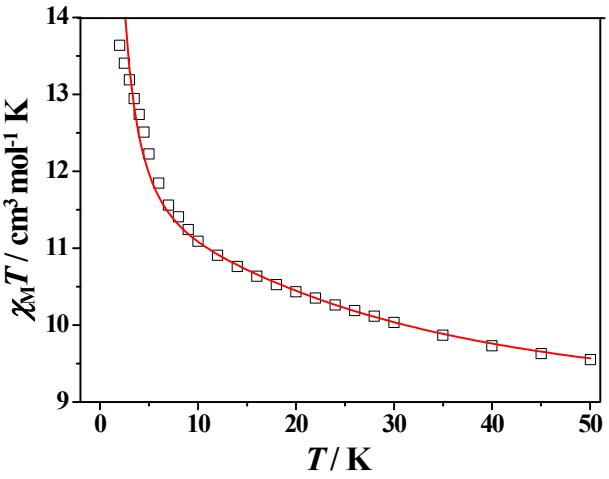


Fig. S11 $\chi_M T$ vs. T (□) plots for complex **4** at the temperature of 0-50 K.

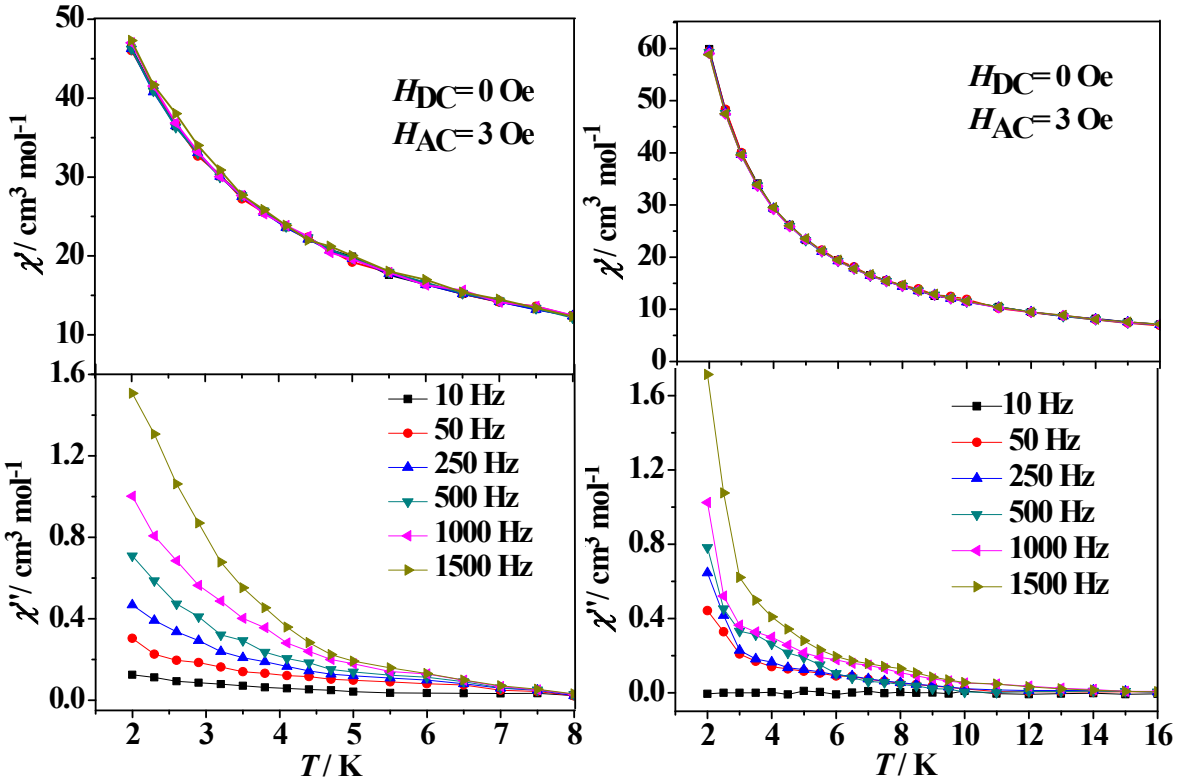


Fig. S12 Temperature dependence of the in-phase(top) and out-of-phase(bottom) components of the AC magnetic susceptibility for complex **5**(left) and **6**(right) in a 0 Oe DC field with an oscillation of 3 Oe.

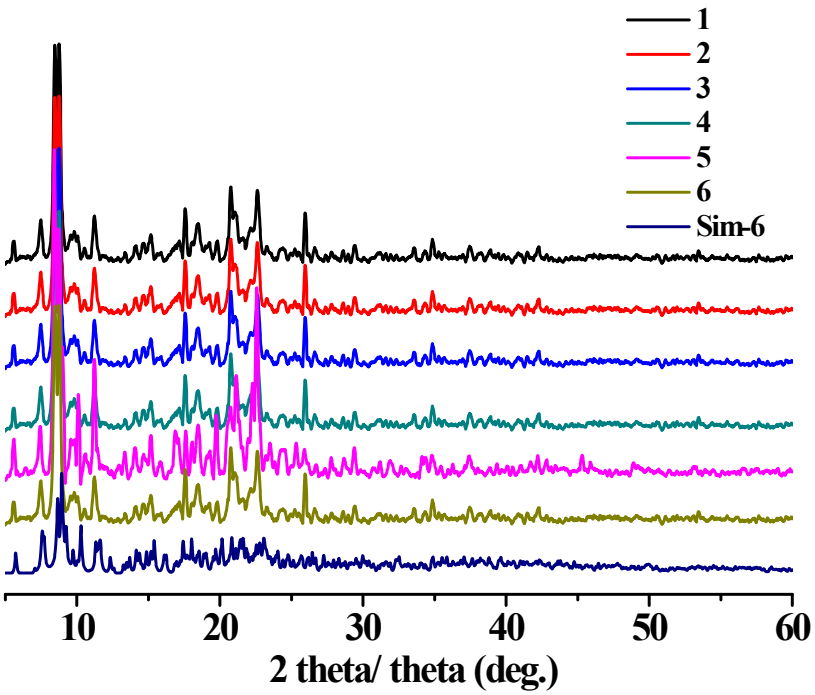


Fig. S13 Powder X-ray diffractions of **1-6**.