Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Modulating spin dynamics of Ln^{III}-radical complexes by using different coligand

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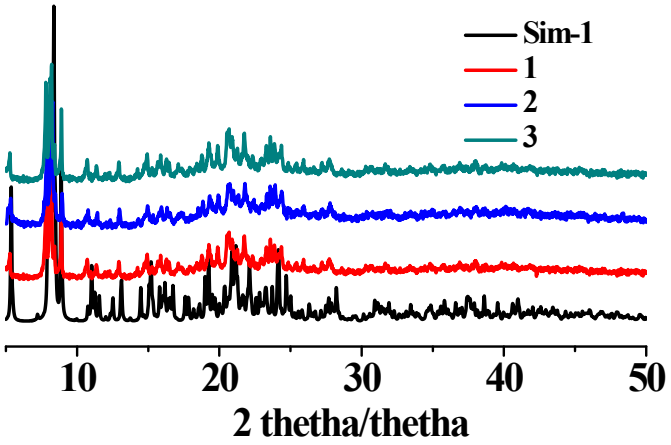

Figure S1. Powder X-ray diffractions of **1-3**.

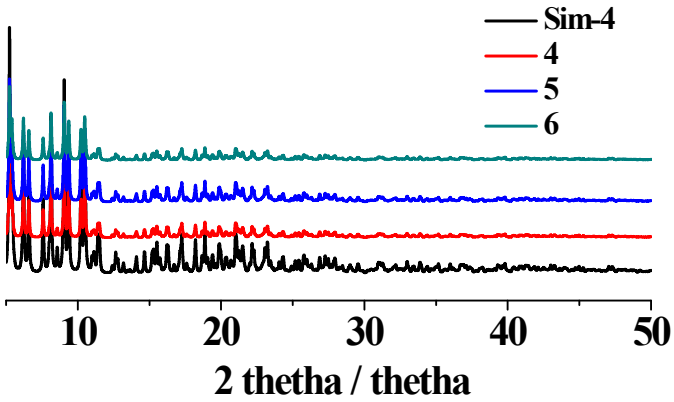

Figure S2. Powder X-ray diffractions of **4-6**.

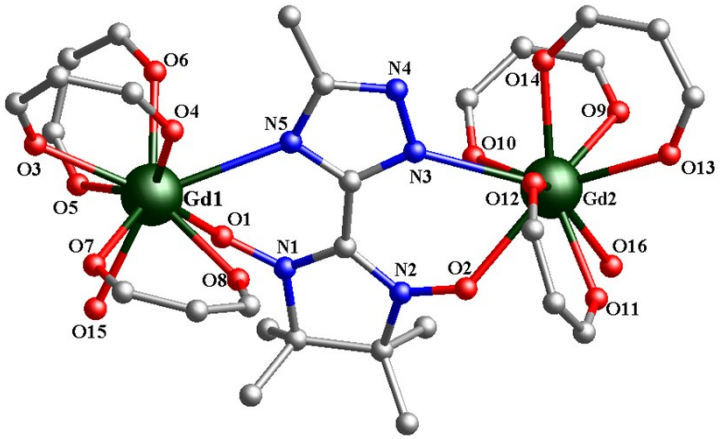

Figure S3. Simplified view of the crystal structure of **1**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

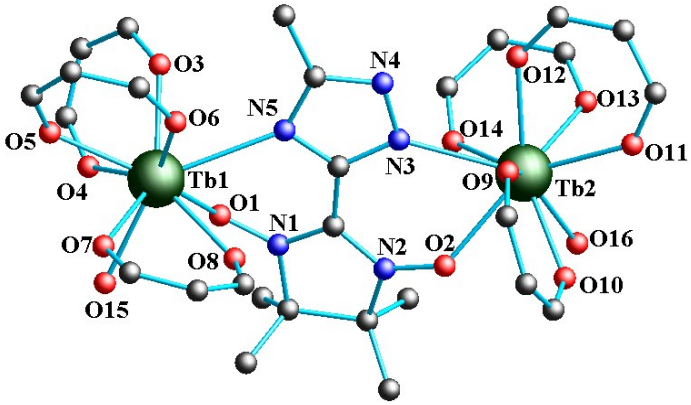

Figure S4. Simplified view of the crystal structure of **2**. Fluorine, hydrogen, and some carbon atoms are omitted for clarity.

Table S1. Selected bond lengths (Å) and bond angles (°) for complex **1**–**4**.

		1	
Dy(1)-O(1)	2.416(5)	O(7)-Dy(1)-O(1)	91.9(2)
Dy(1)-O(3)	2.369(6)	O(4)-Dy(1)-O(1)	139.0(2)
Dy(1)-O(4)	2.350(6)	O(6)-Dy(1)-O(1)	76.22(19)
Dy(1)-O(5)	2.503(6)	O(3)-Dy(1)-O(1)	142.3(2)
Dy(1)-O(6)	2.351(6)	O(8)-Dy(1)-O(1)	70.0(2)
Dy(1)-O(7)	2.337(6)	O(1)-Dy(1)-O(5)	130.9(2)
Dy(1)-O(8)	2.390(6)	O(1)-Dy(1)-N(5)	67.8(2)
Dy(1)-O(15)	2.392(6)	O(4)-Dy(1)-N(5)	71.7(2)
Dy(1)-N(5)	2.698(7)	O(6)-Dy(1)-N(5)	68.1(2)
Dy(2)-O(2)	2.408(6)	N(1)-O(1)-Dy(1)	129.2(5)
Dy(2)-O(9)	2.364(6)	O(9)-Dy(2)-O(2)	74.8(2)
Dy(2)-O(10)	2.478(5)	O(11)-Dy(2)-O(2)	142.3(2)
Dy(2)-O(11)	2.372(6)	O(12)-Dy(2)-O(2)	136.4(2)
Dy(2)-O(12)	2.366(6)	O(14)-Dy(2)-O(2)	66.4(2)
Dy(2)-O(13)	2.353(6)	O(2)-Dy(2)-O(10)	132.6(2)
Dy(2)-O(14)	2.376(6)	O(9)-Dy(2)-N(3)	65.4(2)
Dy(2)-O(16)	2.390(6)	O(2)-Dy(2)-N(3)	67.1(2)
Dy(2)-N(3)	2.625(7)	N(2)-O(2)-Dy(2)	131.6(5)
		2	
Gd(1)-O(1)	2.439(4)	O(3)-Gd(1)-O(1)	142.62(18)
Gd(1)-O(3)	2.390(5)	O(4)-Gd(1)-O(1)	138.93(16)
Gd(1)-O(4)	2.360(5)	O(5)-Gd(1)-O(1)	69.90(16)
Gd(1)-O(5)	2.402(5)	O(6)-Gd(1)-O(1)	91.73(16)
Gd(1)-O(6)	2.353(5)	O(8)-Gd(1)-O(1)	76.56(16)
Gd(1)-O(7)	2.510(5)	O(3)-Gd(1)-N(5)	133.68(17)
Gd(1)-O(8)	2.385(5)	O(4)-Gd(1)-N(5)	71.64(16)
Gd(1)-O(15)	2.416(4)	O(5)-Gd(1)-N(5)	119.22(16)
Gd(1)-N(5)	2.689(5)	O(8)-Gd(1)-N(5)	67.67(16)
Gd(2)-O(2)	2.408(4)	N(1)-O(1)-Gd(1)	128.2(4)
Gd(2)-O(9)	2.497(5)	O(2)-Gd(2)-N(3)	66.87(16)
Gd(2)-O(10)	2.383(5)	O(2)-Gd(2)-O(9)	132.67(16)
Gd(2)-O(11)	2.371(5)	O(2)-Gd(2)-O(16)	77.57(16)
Gd(2)-O(12)	2.363(5)	O(11)-Gd(2)-N(3)	115.82(18)
Gd(2)-O(13)	2.381(4)	O(12)-Gd(2)-N(3)	67.49(17)
Gd(2)-O(14)	2.382(5)	O(13)-Gd(2)-N(3)	133.53(16)
Gd(2)-O(16)	2.411(5)	O(10)-Gd(2)-N(3)	65.33(17)
Gd(2)-N(3)	2.641(6)	N(2)-O(2)-Gd(2)	131.9(4)
		3	
Tb(1)-O(1)	2.424(3)	O(3)-Tb(1)-O(1)	92.06(12)
Tb(1)-O(3)	2.334(4)	O(6)-Tb(1)-O(1)	138.80(12)
Tb(1)-O(4)	2.400(4)	O(8)-Tb(1)-O(1)	76.47(12)

Tb(1)-O(5)	2.376(4)	O(5)-Tb(1)-O(1)	142.34(13)
Tb(1)-O(6)	2.359(4)	O(4)-Tb(1)-O(1)	69.76(12)
Tb(1)-O(7)	2.505(4)	O(1)-Tb(1)-O(7)	130.80(12)
Tb(1)-O(8)	2.367(4)	O(1)-Tb(1)-N(5)	67.87(12)
Tb(1)-O(15)	2.402(3)	O(7)-Tb(1)-N(5)	124.91(13)
Tb(1)-N(5)	2.697(4)	N(1)-O(1)-Tb(1)	128.7(3)
Tb(2)-O(2)	2.407(3)	O(9)-Tb(2)-O(2)	91.14(13)
Tb(2)-O(9)	2.350(4)	O(12)-Tb(2)-O(2)	136.01(12)
Tb(2)-O(10)	2.379(4)	O(14)-Tb(2)-O(2)	74.76(12)
Tb(2)-O(11)	2.372(3)	O(11)-Tb(2)-O(2)	142.70(12)
Tb(2)-O(12)	2.369(3)	O(10)-Tb(2)-O(2)	66.53(12)
Tb(2)-O(13)	2.488(3)	O(2)-Tb(2)-N(3)	67.02(12)
Tb(2)-O(14)	2.371(3)	O(2)-Tb(2)-O(13)	132.44(12)
Tb(2)-O(16)	2.396(4)	O(16)-Tb(2)-O(13)	69.33(12)
Tb(2)-N(3)	2.630(4)	N(2)-O(2)-Tb(2)	132.1(3)
		4	
Gd(1)-O(8)	2.321(6)	O(8)-Gd(1)-O(3)	80.2(2)
Gd(1)-O(3)	2.327(8)	O(8)-Gd(1)-O(5)	75.1(2)
Gd(1)-O(5)	2.338(6)	O(3)-Gd(1)-O(5)	79.8(2)
Gd(1)-O(6)	2.348(6)	O(8)-Gd(1)-O(6)	114.6(2)
Gd(1)-O(4)	2.361(8)	O(3)-Gd(1)-O(6)	141.9(2)
Gd(1)-O(1)	2.368(6)	O(5)-Gd(1)-O(6)	71.5(2)
Gd(1)-O(7)	2.397(7)	O(8)-Gd(1)-O(4)	142.5(3)
Gd(1)-N(1)	2.651(7)	O(8)-Gd(1)-N(1)	79.2(2)
Gd(2)-O(15)	2.332(10)	O(15)-Gd(2)-O(11)	143.6(3)
Gd(2)-O(14)	2.344(8)	O(14)-Gd(2)-O(11)	112.5(2)
Gd(2)-O(11)	2.347(8)	O(15)-Gd(2)-O(12)	79.7(3)
Gd(2)-O(12)	2.350(8)	O(15)-Gd(2)-O(9)	105.8(3)
Gd(2)-O(13)	2.368(6)	O(11)-Gd(2)-O(9)	81.1(3)
Gd(2)-O(9)	2.388(7)	O(15)-Gd(2)-O(16)	73.5(3)
Gd(2)-O(16)	2.406(9)	O(14)-Gd(2)-O(16)	145.8(3)
Gd(2)-N(6)	2.687(8)	O(14)-Gd(2)-N(6)	79.2(2)

Equations for simulating the variable temperature susceptibilities of compound **1:**

$$\chi = \frac{N\beta^2}{12kT} \times [\frac{A}{B}] \tag{1}$$

$$A = 2040 g_{\frac{15}{2},7}^{\ 2} + 1365 g_{\frac{13}{2},7}^2 \exp(\frac{-15J}{kT}) + 1365 g_{\frac{13}{2},6}^2 \exp(\frac{-J-14J'}{kT}) + 858 g_{\frac{11}{2},6}^2 \exp(\frac{-14J-14J'}{kT})$$
$$+ 858 g_{\frac{11}{2},5}^2 \exp(\frac{-2J-26J'}{kT}) + 495 g_{\frac{9}{2},5}^2 \exp(\frac{-13J-26J'}{kT}) + 495 g_{\frac{9}{2},4}^2 \exp(\frac{-3J-36J'}{kT}) +$$
$$252 g_{\frac{7}{2},4}^2 \exp(\frac{-12J-36J'}{kT}) + 252 g_{\frac{7}{2},3}^2 \exp(\frac{-4J-44J'}{kT}) + 105 g_{\frac{5}{2},3}^2 \exp(\frac{-11J-44J'}{kT}) +$$
$$105 g_{\frac{5}{2},2}^2 \exp(\frac{-5J-50J'}{kT}) + 30 g_{\frac{3}{2},2}^2 \exp(\frac{-10J-50J'}{kT}) + 30 g_{\frac{3}{2},1}^2 \exp(\frac{-6J-54J'}{kT}) +$$
$$3 g_{\frac{1}{2},1}^2 \exp(\frac{-9J-54J'}{kT}) + 3 g_{\frac{1}{2},0}^2 \exp(\frac{-7J-56J'}{kT})$$

$$B = 8 + 7\exp(\frac{-15J}{kT}) + 7\exp(\frac{-J-14J'}{kT}) + 6\exp(\frac{-14J-14J'}{kT}) + 6\exp(\frac{-2J-26J'}{kT}) +$$
$$5\exp(\frac{-13J-26J'}{kT}) + 5\exp(\frac{-3J-36J'}{kT}) + 4\exp(\frac{-12J-36J'}{kT}) + 4\exp(\frac{-4J-44J'}{kT}) +$$
$$3\exp(\frac{-11J-44J'}{kT}) + 3\exp(\frac{-5J-50J'}{kT}) + 2\exp(\frac{-10J-50J'}{kT}) + 2\exp(\frac{-6J-54J'}{kT}) +$$
$$\exp(\frac{-9J-54J'}{kT}) + \exp(\frac{-7J-56J'}{kT})$$

$$g_{\frac{15}{2},7} = \frac{238 g_{Gd} + 17 g_R}{255}, \qquad g_{\frac{13}{2},7} = \frac{208 g_{Gd} - 13 g_R}{195}, \qquad g_{\frac{13}{2},6} = \frac{60 g_{Gd} + 5 g_R}{65},$$

$$g_{\frac{11}{2},6} = \frac{154 g_{Gd} - 11 g_R}{143}, \qquad g_{\frac{9}{2},5} = \frac{108 g_{Gd} - 9 g_R}{99}, \qquad g_{\frac{9}{2},4} = \frac{88 g_{Gd} + 11 g_R}{99},$$

$$g_{\frac{7}{2},4} = \frac{70 g_{Gd} - 7 g_R}{63}, \qquad g_{\frac{7}{2},3} = \frac{54 g_{Gd} + 9 g_R}{63}, \qquad g_{\frac{5}{2},3} = \frac{40 g_{Gd} - 5 g_R}{35},$$

$$g_{\frac{5}{2},2} = \frac{28 g_{Gd} + 7 g_R}{35}, \qquad g_{\frac{3}{2},2} = \frac{18 g_{Gd} - 3 g_R}{15}, \qquad g_{\frac{3}{2},1} = \frac{2 g_{Gd} + g_R}{3},$$

$$g_{\frac{1}{2},1} = \frac{4 g_{Gd} - g_R}{3}, \qquad g_{\frac{1}{2},0} = g_R,$$

$$\chi_M T = \frac{\chi T}{1 - (2zj'/Ng^2\beta^2)\chi} \tag{2}$$

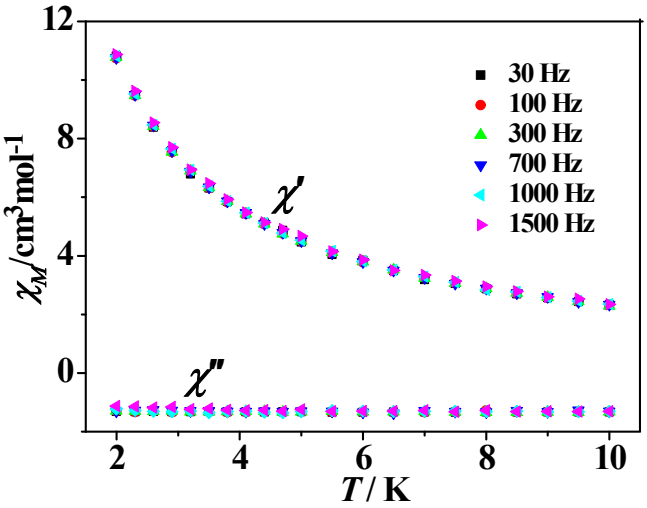

Figure S5. Temperature dependence of the imaginary of the in-phase (χ′) and out-of-phase (χ″) components of the AC magnetic susceptibility for complex **2** in zero applied field in the range 30 Hz to 1500 Hz.

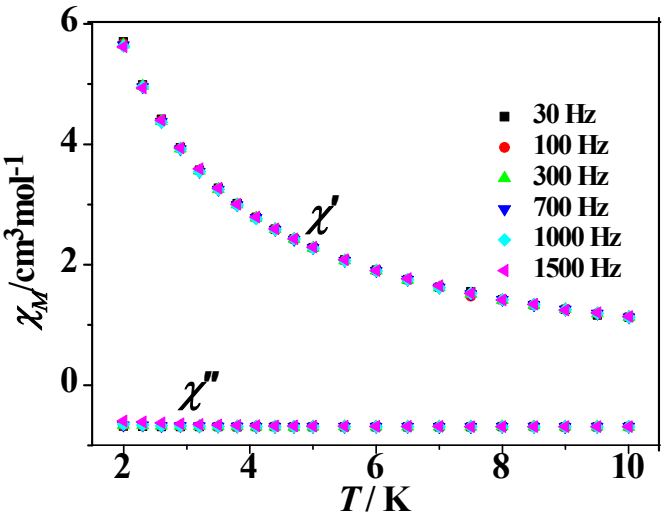

Figure S6. Temperature dependence of the imaginary of the in-phase (χ′) and out-of-phase (χ″) components of the AC magnetic susceptibility for complex **6** in zero applied field in the range 30 Hz to 1500 Hz.