Electronic supplementary information (ESI)

Chiral six-coordinate Dy(III) and Tb(III) complexes of an achiral ligand: Structure, fluorescence, and magnetism

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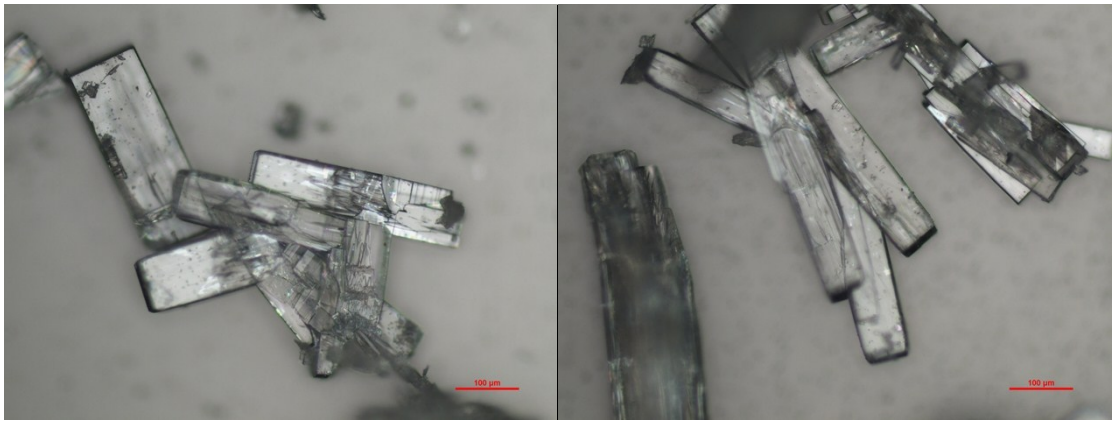

Fig. S1. Crystals under ordinary microscope for complexes **1** (left) and **2** (right).

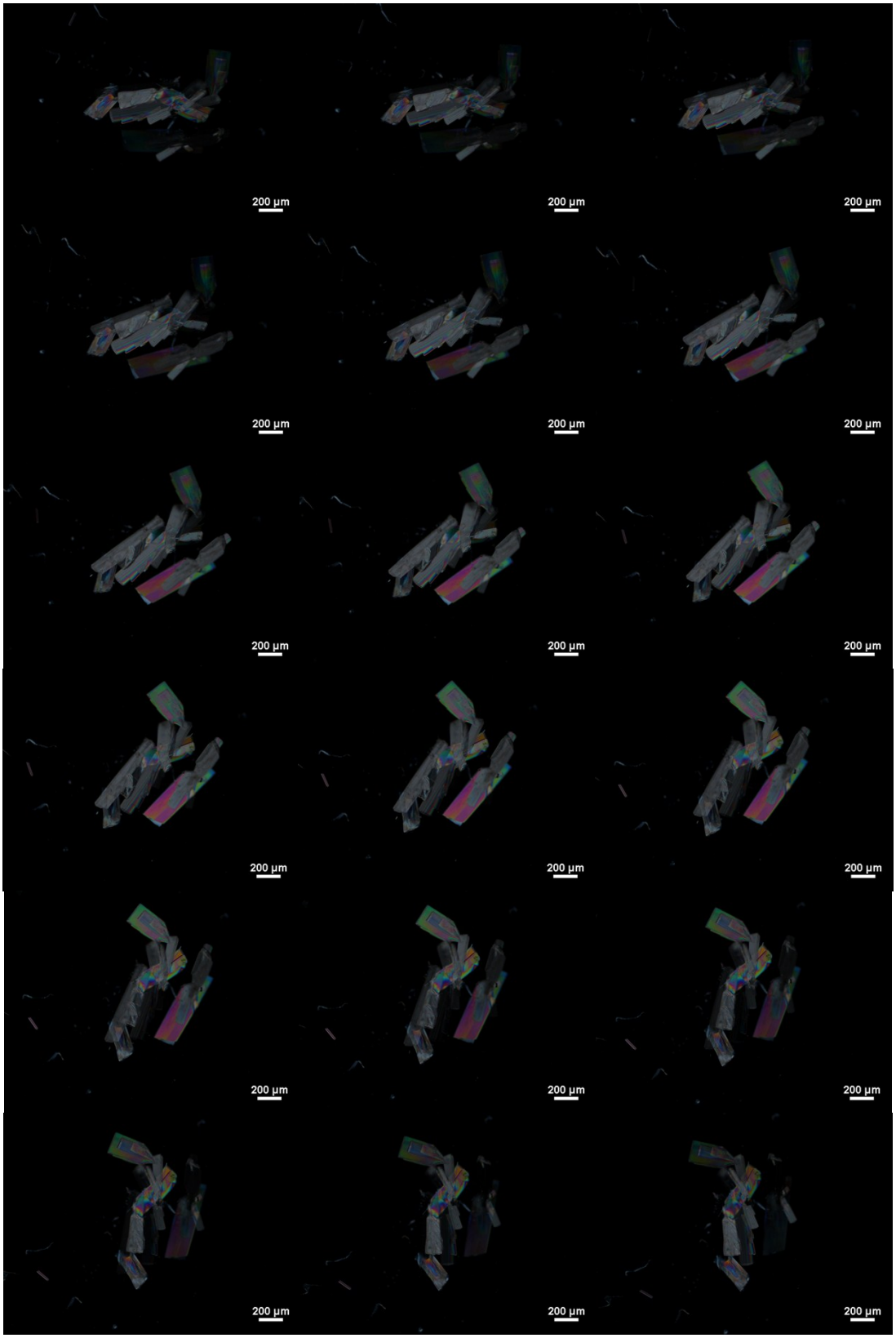

Fig. S2. Crystals under polarizing microscope from 0° to 85° for complex **1** (five degrees apart).

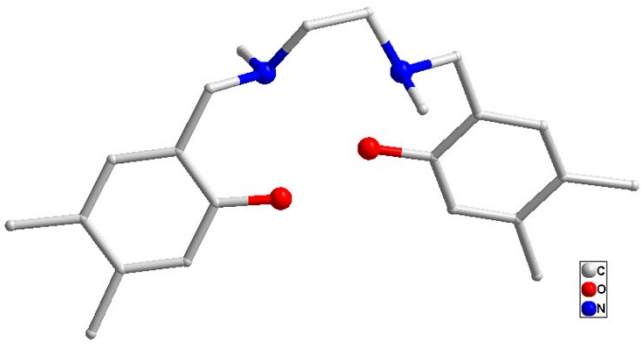

Fig. S3. Crystal structure of the ligand. Hydrogens have been omitted for clarity.

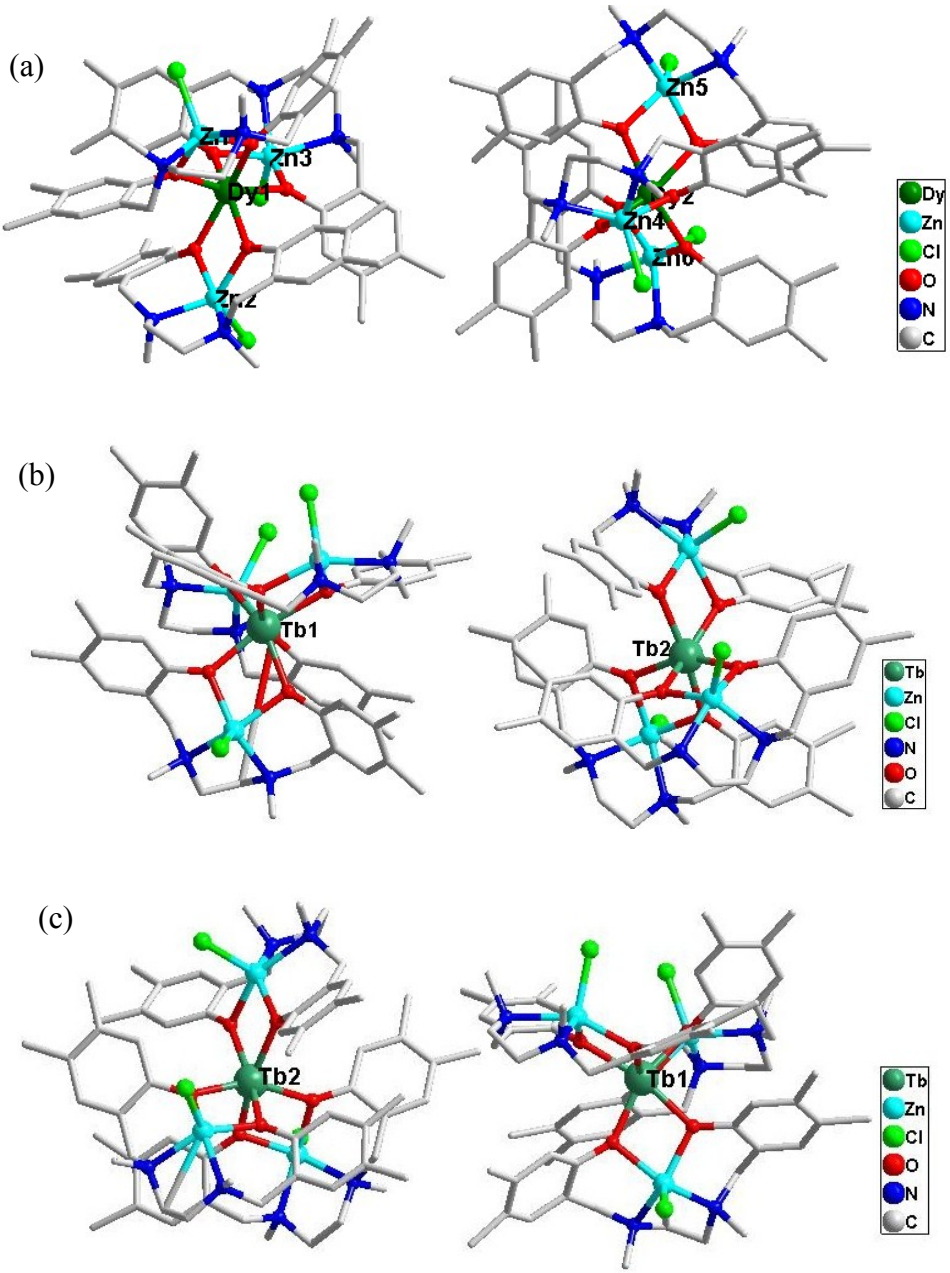

Fig. S4. Main molecular structure of complexes *Λ*-**1** (a), *Λ*-**2** and *Δ*-**2** (c). Hydrogens and solvents have been omitted for clarity.

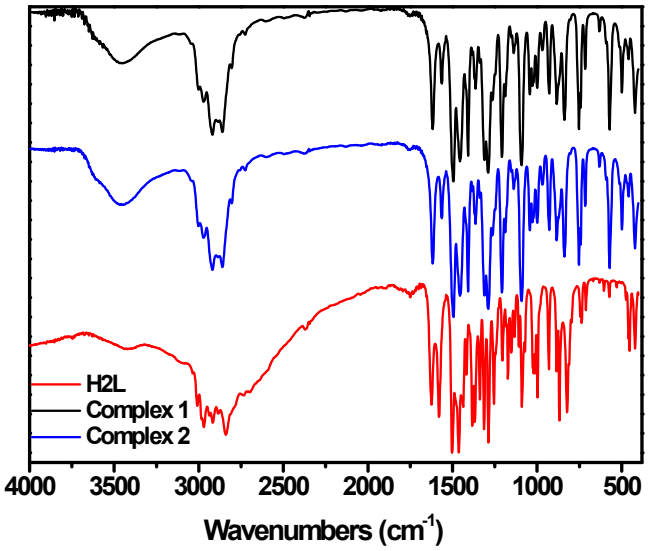

Fig. S5. The IR spectra for the ligand H_2L (red), complex **1** (black) and **2** (blue).

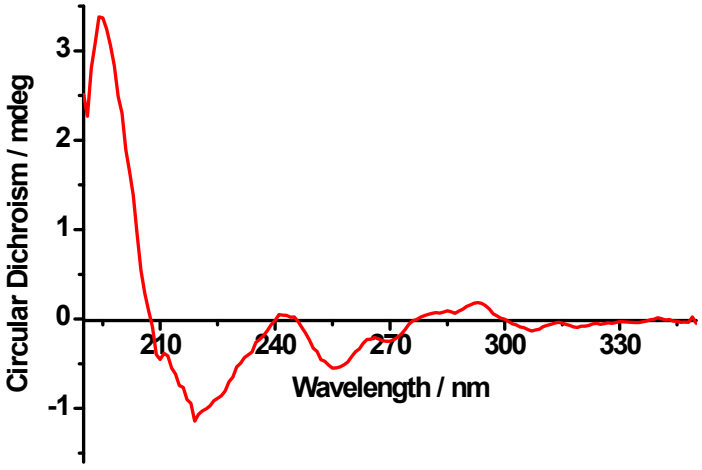

Fig. S6. The solution circular dichroism (CD) spectrum in methanol for complex **1** (100 μmol/L).

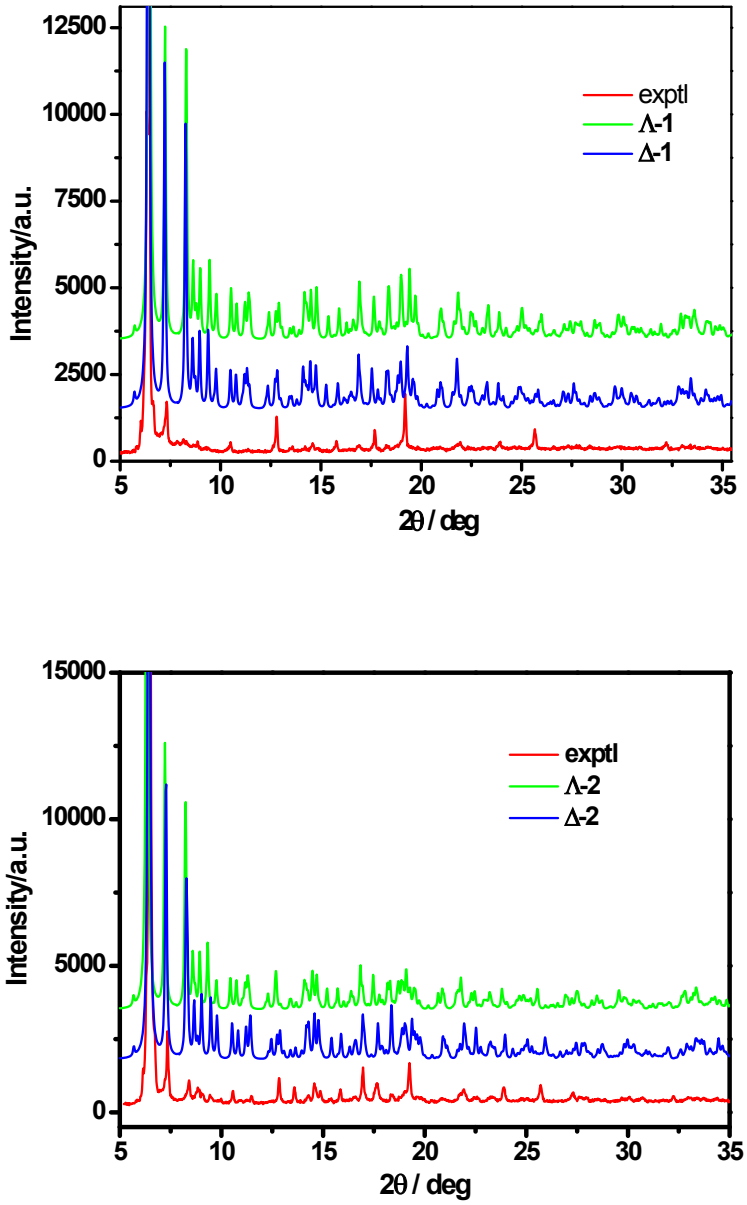

Fig. S7. Powdered X-ray diffraction (XRD) patterns for complexes **1** and **2**.

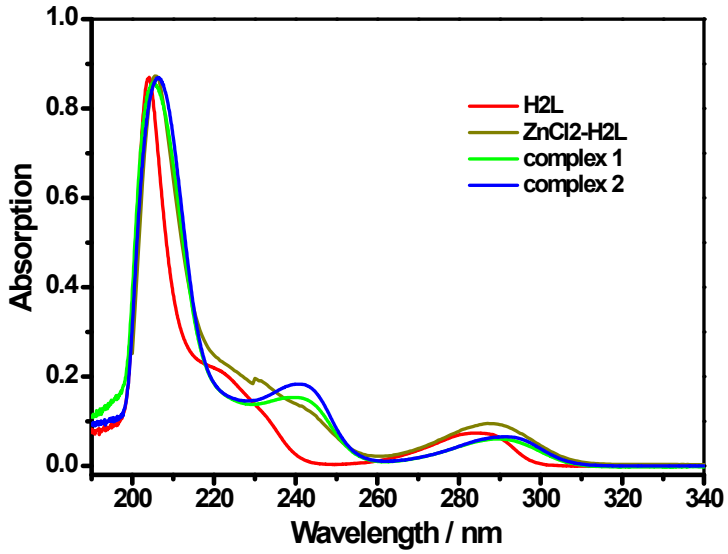

Fig. S8. The solution UV-Vis spectroscopies in methanol for the ligand (red), $ZnCl_2$-H_2L (brown), complex **1** (green) and complex **2** (blue).

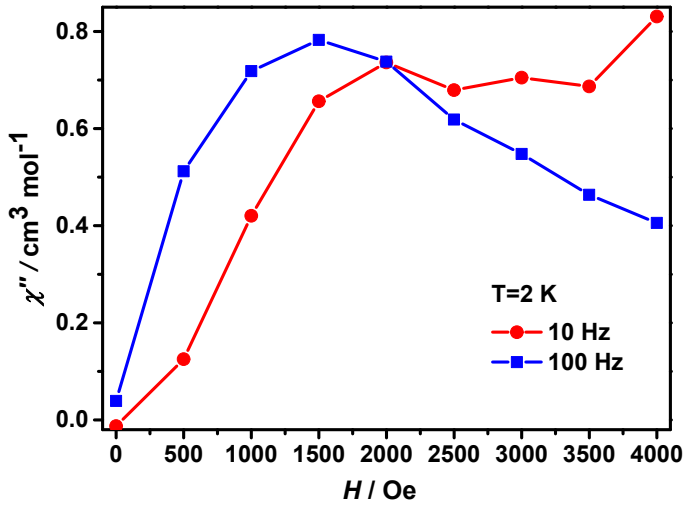

Fig. S9. The out-of-phase component (χ") vs. external dc field (H) for complex **1** at 2 K with an oscillation of 2.0 Oe and frequencies of 10 Hz and 100 Hz.

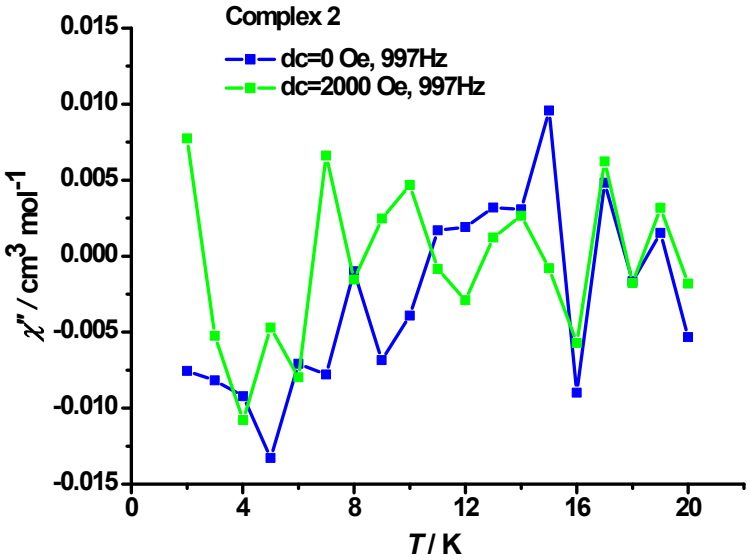

Fig. S10. Temperature dependence of the out-of-phase component (χ") for complex **2** at 997 Hz.

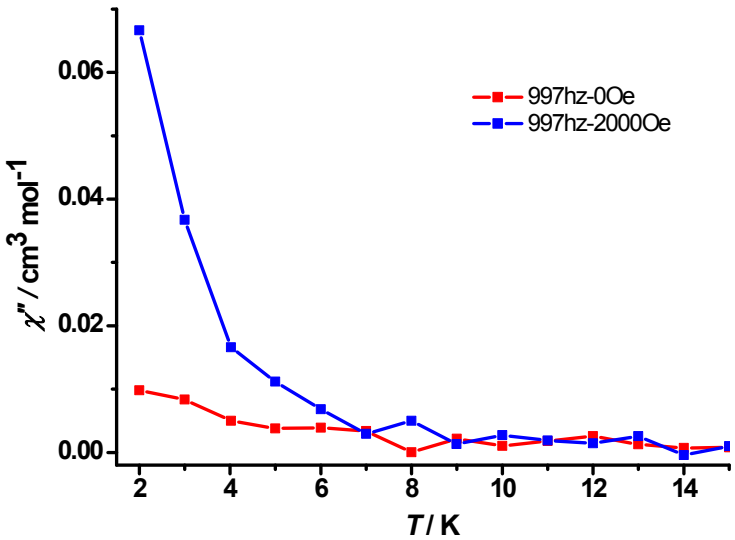

Fig. S11. Temperature dependence of the out-of-phase component (χ") for diluted sample ($Dy_{0.05}Y_{0.95}$) of complex **1** at 997 Hz.

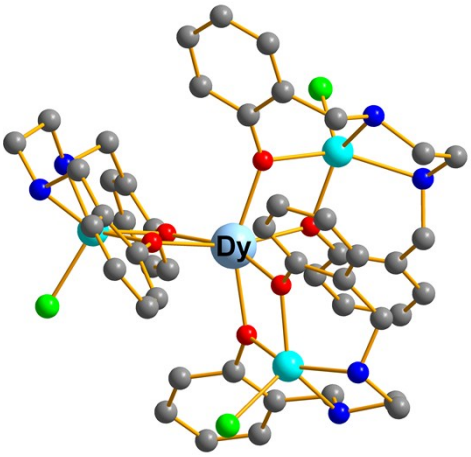

Fig. S12. Calculated complete structure of complex **1**; H atoms are omitted.

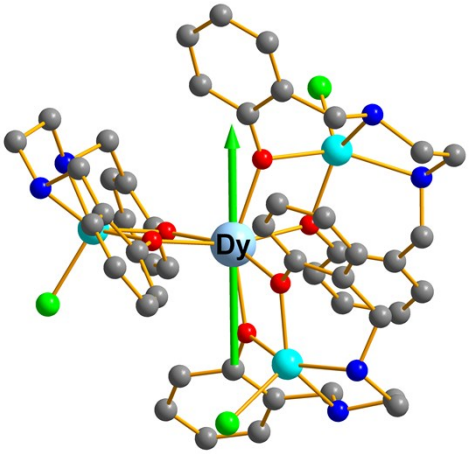

Fig. S13. Orientation of the local main magnetic easy axis of the ground Kramers doublet on Dy^{III} of complex **1**.

Table S1. Calculation results of the lowest Kramers doublets (KDs) of Dy^{III} for complex **1**.

KDs	**Complex 1**			
	E/cm^{-1}	***g***		m_J
1	0.0	g_x	0.089	±15/2
		g_y	3.935	
		g_z	15.492	
2	35.2	g_x	0.339	±3/2
		g_y	3.069	
		g_z	14.160	
3	71.8	g_x	0.540	±1/2
		g_y	1.310	
		g_z	16.026	
4	169.7	g_x	6.386	±5/2
		g_y	6.797	
		g_z	7.993	
5	294.6	g_x	0.686	±11/2

		g_y	2.376	
		g_z	11.548	
6	318.5	g_x	0.306	±13/2
		g_y	1.562	
		g_z	12.414	
7	376.0	g_x	1.182	±7/2
		g_y	2.030	
		g_z	16.048	
8	543.9	g_x	0.013	±9/2
		g_y	0.035	
		g_z	19.105	

Table S2. In wave functions with definite projection of the total moment $|m_J>$ for the lowest two Kramers doublets (KDs) of the Dy^{III} for complex **1**.

	***E*/cm^{-1}**	**wave functions**
1	0.0	72%|±15/2> + 5%|±7/2> + 5%|±3/2> + 10%|±1/2>
	35.1	17%|±15/2> + 5%|±13/2> + 13%|±5/2> + 24%|±3/2> + 35%|±1/2>