Supporting Information

Phthalocyanine supported dinuclear Ln^{III} complexes: the solvent-induced change of magnetic properties in dysprosium(III) analogue

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Table S1 Selected bond lengths (Å) and bond angles (°) for **1**−**3**

	1 (Sm_2-C_6H_6)	**2** (Tb_2-C_6H_6)	**3** (Dy_2-C_6H_6)
Bond Lengths (Å)			
Ln1—O1	2.300 (3)	2.255(3)	2.249(3)
Ln1—O2	2.281 (3)	2.250(3)	2.235(3)
Ln1—N1	2.674 (4)	2.641(5)	2.628(5)
Ln1—N1A	2.649 (4)	2.613(5)	2.606(5)
Ln1—N3	2.655(3)	2.618(3)	2.601(4)
Ln1—Ln1A	3.6109 (6)	3.5383(6)	3.5121(7)
Bond Angles (°)			
O2—Ln1—O2B	73.85 (17)	74.52 (16)	74.65 (19)
O2—Ln1—O1	80.29 (11)	79.24 (12)	78.78 (13)
O2—Ln1—O1B	123.18 (11)	123.22 (12)	122.95 (14)
O1—Ln1—O1B	73.16 (17)	74.70 (17)	75.04(19)
O2—Ln1—N3	139.76 (8)	140.06 (8)	140.20(10)
O1—Ln1—N3	139.56 (8)	140.30 (8)	140.63(10)
O2—Ln1—N3A	83.25 (9)	82.78 (10)	82.75(11)
O1—Ln1—N3A	83.52 (10)	82.82 (10)	82.79(11)
N3—Ln1—N3A	94.31 (13)	94.97 (14)	95.06(16)
O2—Ln1—N1A	142.66 (8)	142.41 (8)	142.37(9)
O1—Ln1—N1A	81.04 (11)	81.15 (12)	81.36(13)
N3—Ln1—N1A	62.70 (7)	63.12 (7)	63.21(8)
O2—Ln1—N1	81.59 (11)	81.45 (12)	81.38(13)
O1—Ln1—N1	142.91 (9)	142.26 (8)	142.17(10)
N3—Ln1—N1	62.70 (7)	62.74 (7)	62.91 (8)
N1A—Ln1—N1	94.57 (12)	95.34 (13)	95.70 (15)
O2—Ln1—Ln1A	118.35 (7)	118.31 (8)	118.39 (10)
O1—Ln1—Ln1A	118.46 (8)	118.47 (8)	118.66 (10)
N3—Ln1—Ln1A	47.15 (7)	47.48 (7)	47.53 (8)
N1A—Ln1—Ln1AA	47.58 (9)	48.01 (10)	48.12 (12)
N1—Ln1—Ln1A	46.99 (10)	47.34 (10)	47.59 (11)
Ln1A—N1—Ln1	85.43 (12)	84.66 (13)	84.30 (15)

Ln1—N3—Ln1A	85.69 (13)	85.03 (14)	84.94 (16)

Symmetry codes: (A) -*x*+1, -*y*+1, -*z*; (B) *x*, -*y*+1, *z*.

Table S2 Crystal data and structure refinement for **1′** [S1]

	1′
Empirical formula	$C_{76}H_{92}N_8O_8Sm_2$
Formula weight	1546.29
Crystal system	Triclinic
Space group	$P\bar{1}$
a (Å)	12.941(6)
b (Å)	14.680(4)
c (Å)	21.205(4)
α (°)	88.22(2)
β (°)	86.54(3)
γ (°)	71.32(3)
V (Å^3)	3808.94
Z	2
ρ calc (g/cm^3)	1.267
F(000)	1400

Table S3 Fitting of the Cole-Cole plots for **3** with a generalized Debye model in the temperature range 2.6–6.8 K under 1000 Oe dc field.

T / K	χ_s / cm^3 mol^{-1}	χ_T / cm^3 mol^{-1}	*α*
2.6	0.380	12.8	0.39
2.8	0.481	11.7	0.37
3.0	0.551	10.7	0.34
3.2	0.586	9.83	0.32
3.4	0.652	9.12	0.29
3.6	0.651	8.60	0.29
3.8	0.700	8.12	0.28
4.0	0.707	7.81	0.28
4.2	0.732	7.42	0.29
4.4	0.853	7.04	0.29

4.6	0.980	6.75	0.28
4.8	1.17	6.44	0.27
5.0	1.24	6.17	0.26
5.2	1.42	5.90	0.25
5.4	1.52	5.69	0.25
5.6	1.59	5.48	0.26
5.8	1.73	5.29	0.25
6.2	1.87	4.95	0.23
6.8	1.10	4.50	0.18

Table S4 Fitting of the Cole-Cole plots for **3′** with an extended Debye model in the temperature range 3.6–7.2 K under 2000 Oe dc field.

T / K	χ_T / cm^3 mol^{-1}	χ_0 / cm^3 mol^{-1}	ln τ_1	α_1	ln τ_2	α_2
3.6	6.06	0.94	-5.01	0.27	-1.90	0.04
3.9	6.01	0.94	-6.06	0.25	-2.28	0.13
4.2	5.75	0.86	-6.94	0.25	-2.76	0.15
4.5	5.45	0.72	-7.89	0.29	-3.27	0.18
4.8	5.06	0.01	-9.15	0.45	-3.79	0.13
5.1	4.79	0.00			-4.41	0.11
5.7	4.37	2.19			-5.96	0.26
6.0	4.14	2.23			-6.74	0.19
6.3	3.92	2.21			-7.36	0.15
6.6	3.76	2.16			-7.94	0.15
7.0	3.60	2.09			-8.61	0.13
7.2	3.47	1.83			-9.43	0.17

Table S5 Fitting of the Cole-Cole plots for **3-re** with a generalized Debye model in the temperature range 3.0–5.6 K under 1000 Oe dc field.

T / K	χ_S / cm^3 mol^{-1}	χ_T / cm^3 mol^{-1}	α
3.0	0.671	11.1	0.35
3.6	0.787	8.99	0.29
4.0	0.803	8.08	0.28

4.6	1.06	6.98	0.28
5.0	1.32	6.39	0.27
5.6	1.72	5.69	0.26

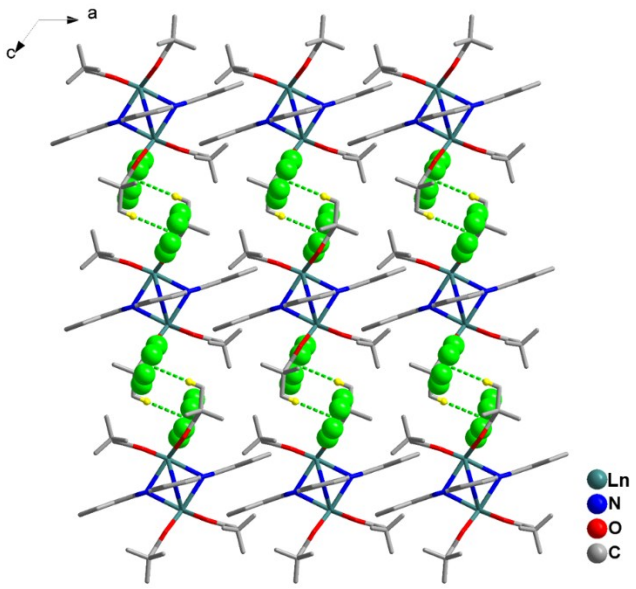

Fig. S1 The benzene molecules lie in crystal lattice regularly in complexes **1**–**3**. The C−H···π interactions and benzene molecules are shown in green dashed lines and space-filling model, respectively.

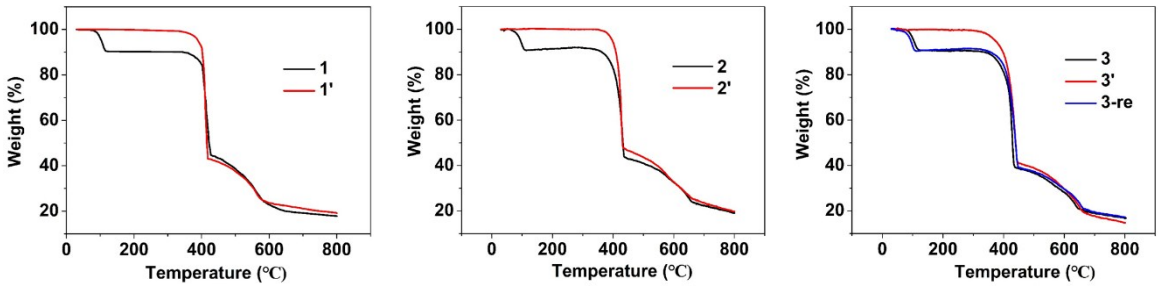

Fig. S2 TGA curves for complexes **1**–**3**, **1′**–**3′** and **3-re**.

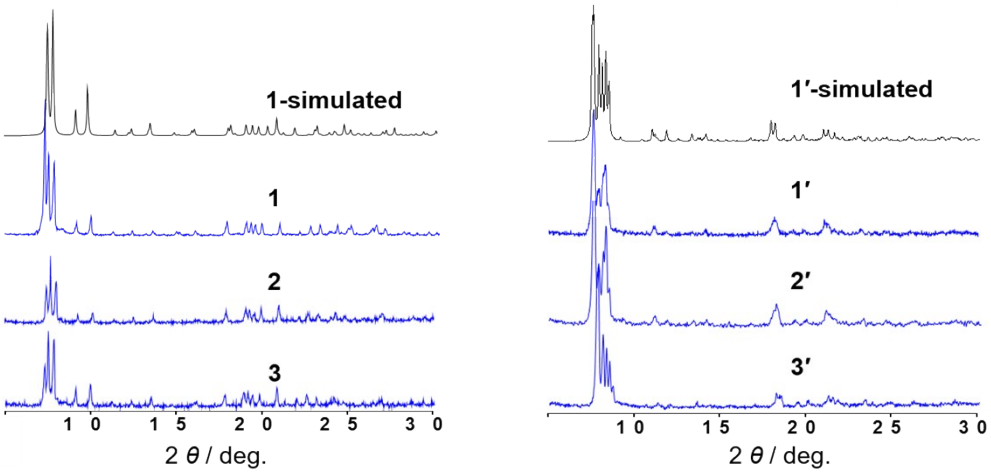

Fig. S3 PXRD patterns. Black: simulated PXRD pattern based on Sm complexes **1** and **1′**. Blue: measured PXRD patterns based on **1**–**3** and **1′**–**3′**.

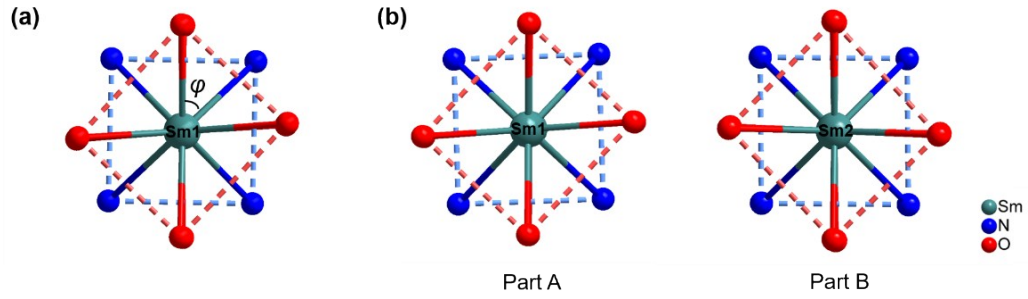

Fig. S4 Some structural parameters change after desolvation, and there are also some different parameters between part A and part B, exspecially the twist angle φ. Taking two Sm complexes for example, three φ values in the order of this graphics are 42.87 (Sm1 for **1**), 42.02 (Sm1 of **1′**) and 44.19 (Sm2 of **1′**), respectively.

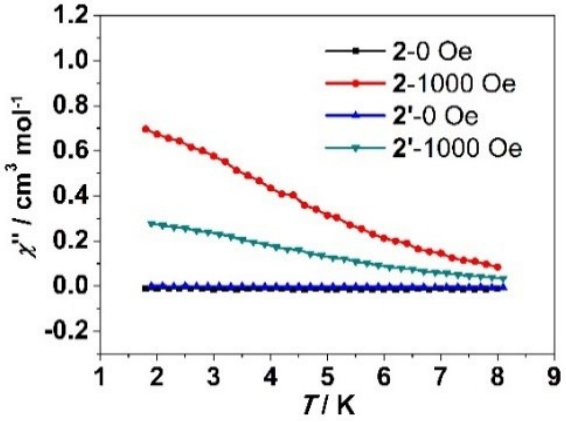

Fig. S5 Temperature dependence of the χ'' ac susceptibilities at 999 Hz under zero and 1000 Oe dc field for **2** and **2′**.

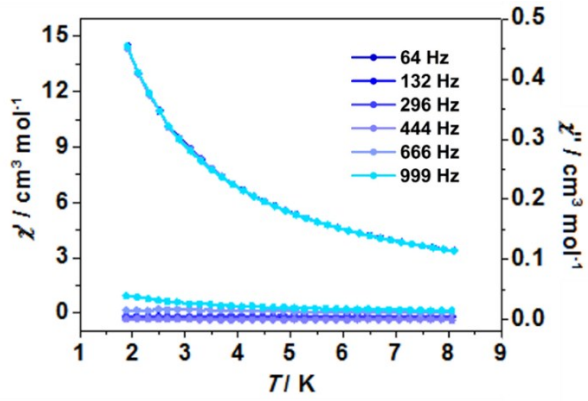

Fig. S6 Temperature dependence of the χ' and χ'' ac susceptibilities at indicated frequencies under zero dc field for **3**.

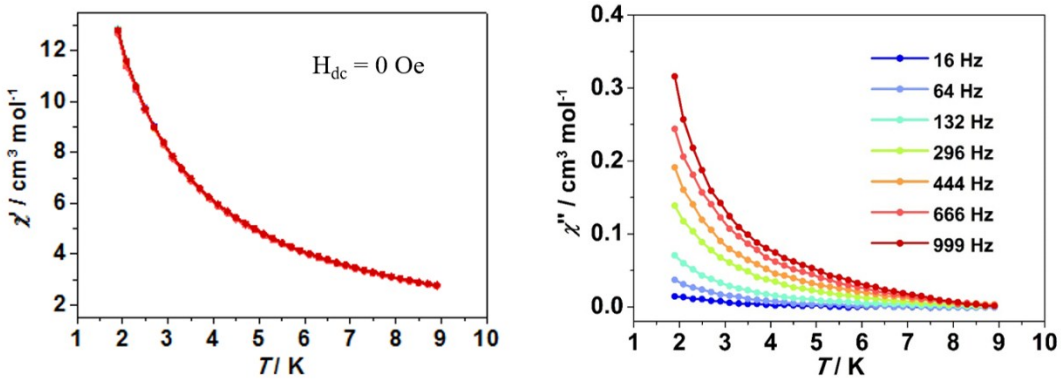

Fig. S7 Temperature dependence of the χ' and χ'' ac susceptibilities at indicated frequencies under zero dc field for **3′**.

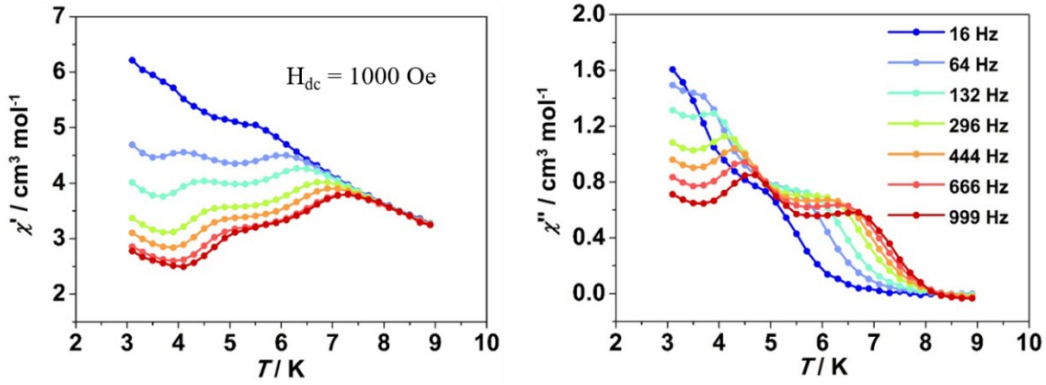

Fig. S8 Temperature dependence of the χ' and χ'' ac susceptibilities at indicated frequencies under 1000 Oe dc field for **3′**.

Reference

[S1] H. Sugimoto, T. Higashi, A. Maeda, M. Mori, H. Masuda and T. Taga, *J. Chem. Soc. Chem. Commun.*, 1983, 1234-1235.