

Supporting Information

Magnetic Properties and Structure of Tetranuclear Lanthanide Complexes Based on 8-hydroxylquinoline Schiff Base Derivative and β -diketone coligand

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Table S1. The important bond lengths [Å] and angles [°] for **1**

<i>Bond distances</i>			
Gd1-Gd2	3.6056 (6)	Gd1a-Gd2	3.8970(8)
Gd1-Gd2a	3.8970(8)	Gd2-Gd2a	3.8722(9)
Gd1-O4	2.337(5)	Gd1-O5	2.353(5)
Gd2a-O8	2.357(5)	Gd1-O1	2.408(5)
Gd1-O8	2.346(5)	Gd1-O3	2.403(5)
Gd2-O8	2.412(5)	Gd1-O2	2.407(5)
Gd2-N1a	2.581(6)	Gd2-O7	2.339(5)
Gd2-O8a	2.357(5)	Gd2-O6	2.326(5)
Gd2-O3	2.402(5)	Gd2-O2	2.437(5)
Gd2-O1a	2.388(5)	Gd1-N5	2.560(6)
Gd1-N3	2.549(6)	Gd2a-O1	2.388(5)
Gd2a-N1	2.581(6)		
<i>Angles</i>			
Gd1-Gd2-Gd2a	62.699(14)	Gd2-Gd1-Gd2a	62.000(14)
Gd1-Gd2-Gd1a	117.998(14)	Gd1a-Gd2-Gd2a	55.299(11)
Gd1-O1-Gd2a	108.68(18)	Gd1-O2-Gd2	95.95(17)
Gd1-O3-Gd2	97.24(16)	Gd1-O8-Gd2a	111.92(19)
Gd2-O8-Gd2a	108.56(18)	Gd1-O8-Gd2	98.54(18)

Table S2. The important bond lengths [Å] and angles [°] for **2**

<i>Bond distances</i>			
Tb1-Tb2	3.5897(3)	Tb1a- Tb2	3.8852(3)
Tb1- Tb2a	3.8852(3)	Tb2- Tb2a	3.8489(4)
Tb1-O4	2.319(3)	Tb1-O5	2.337(3)
Tb2-O8	2.392(3)	Tb1-O1	2.407(3)
Tb1-O8	2.339(3)	Tb1-O3	2.388(3)
Tb2a-O8	2.346(3)	Tb1-O2	2.386(3)
Tb2-N1a	2.553(3)	Tb2-O7	2.318(3)
Tb2-O8a	2.346(3)	Tb2-O6	2.335(3)
Tb2-O3	2.427(3)	Tb2-O2	2.392(3)
Tb2-O1a	2.385(3)	Tb1-N7	2.565(4)
Tb1-N4	2.557(4)	Tb2a-O1	2.385(3)
Tb2a-N1	2.553(3)		
<i>Angles</i>			
Tb1-Tb2-Tb1a	118.167(6)	Tb2-Tb1-Tb2a	61.832(6)
Tb1-Tb2-Tb2a	62.861(6)	Tb1a-Tb2-Tb2a	55.306(6)
Tb1-O1-Tb2a	108.34(10)	Tb1-O2-Tb2	97.4(1)
Tb1-O3-Tb2	96.4(1)	Tb1-O8-Tb2a	112.04(11)
Tb2-O8-Tb2a	108.64(10)	Tb1-O8-Tb2	98.71(11)

Table S3. The important bond lengths [Å] and angles [°] for **3**

<i>Bond distances</i>			
Dy1-Dy2	3.5621 (3)	Dy1-Dy1a	3.8194(5)
Dy1-Dy2a	3.8628(4)	Dy1a-Dy2	3.8628(4)
Dy1-O4	2.303(3)	Dy1-O5	2.320(3)
Dy1-O8a	2.332(3)	Dy1-O1	2.366(3)
Dy1-O8	2.367(3)	Dy1-O3	2.379(3)
Dy1a-O8	2.332(3)	Dy1-O2	2.417(3)
Dy1-N1	2.540(4)	Dy2-O7	2.305(3)
Dy2-O8	2.335(3)	Dy2-O6	2.320(3)
Dy2-O3	2.363(3)	Dy2-O2	2.376(3)
Dy2-O1a	2.393(3)	Dy2-N7	2.537(4)
Dy2-N4	2.551(4)	Dy2a-O1	2.393(3)
<i>Angles</i>			
Dy1-Dy2-Dy1a	61.758(7)	Dy2-Dy1-Dy2a	118.243(7)
Dy1a-Dy1-Dy2a	55.247(6)	Dy2-Dy1-Dy1a	62.996(7)
Dy1-O1-Dy2a	108.52(11)	Dy1-O2-Dy2	96.02(11)
Dy1-O3-Dy2	97.38(10)	Dy1a-O8-Dy2	111.73(11)
Dy1-O8-Dy1a	108.73(11)	Dy1-O8-Dy2	98.51(11)

Table S4. The important bond lengths [Å] and angles [°] for **4**

<i>Bond distances</i>			
Ho1-Ho2	3.5508(4)	Ho1-Ho1a	3.8062(5)
Ho1-Ho2a	3.8503(5)	Ho1a-Ho2	3.8504(5)
Ho1-O4	2.302(3)	Ho1-O5	2.313(4)
Ho1-O8a	2.320(3)	Ho1-O1	2.367(3)
Ho1-O8	2.370(3)	Ho1-O3	2.372(3)
Ho1a-O8	2.320(3)	Ho1-O2	2.403(3)
Ho1-N1	2.532(4)	Ho2-O7	2.303(3)
Ho2-O8	2.323(3)	Ho2-O6	2.316(4)
Ho2-O3	2.361(3)	Ho2-O2	2.365(3)
Ho2-O1a	2.382(4)	Ho2-N7	2.529(4)
Ho2-N4	2.541(4)	Ho2a-O1	2.382(4)
<i>Angles</i>			
Ho1-Ho2-Ho1a	61.740(9)	Ho2-Ho1-Ho2a	118.260(9)
Ho1a-Ho1-Ho2	63.003(9)	Ho1a- Ho1-Ho2a	55.257(7)
Ho1-O1-Ho2a	108.32(13)	Ho1-O2-Ho2	96.24(12)
Ho1-O3-Ho2	97.21(12)	Ho1a-O8- Ho2	112.06(13)
Ho1-O8- Ho1a	108.49(13)	Ho1-O8- Ho2	98.32 (13)

Table S5. The important bond lengths [Å] and angles [°] for **5**

<i>Bond distances</i>			
Er1-Er2	3.5355(3)	Er1a-Er2	3.8354(3)
Er1-Er2a	3.8355(3)	Er2-Er2a	3.7900(4)
Er1-O4	2.298(3)	Er1-O5	2.308(3)
Er2-O8a	2.360(2)	Er1-O1	2.368(3)
Er1a-O8	2.306(3)	Er1-O3	2.356(3)
Er1-O8a	2.306(3)	Er1-O2	2.355(3)
Er2-N1a	2.520(3)	Er2-O7	2.308(3)
Er2-O8	2.313(2)	Er2-O6	2.292(2)
Er2-O3	2.399(2)	Er2-O2	2.363(3)
Er2-O1a	2.354(3)	Er1-N7	2.534(3)
Er1-N4	2.517(3)	Er2a-O1	2.354(3)
Er2a-O8	2.369(2)		
<i>Angles</i>			
Er1-Er2-Er1a	118.27(1)	Er2-Er1-Er2a	61.73(1)
Er1a-Er2-Er2a	55.240	Er1-Er2-Er2a	63.03(1)
Er1-O1-Er2a	108.62(10)	Er1-O2-Er2	97.07(9)
Er1-O3-Er2	96.08(8)	Er1a-O8-Er2	112.27(10)
Er2-O8-Er2a	108.41(9)	Er1a-O8-Er2a	98.53(9)

Table S6. Comparison of some important bond lengths and bond angles

Aromatic aldehyde and β -diketonate	Dy-O (Å)	Dy-N (Å)	Dy...Dy (shortest) (Å)	α angle (°)	O-Dy-O (°)	Ref.
4-pyridinecarboxaldehyde Dy(dbm)₃·2H₂O	2.303(3)-2.417(3)	2.537(4)-2.551(4)	3.5621(3)	51.41-65.09	67.71(10)-145.13(10)	this work
4-fluorobenzaldehyde Dy(dbm) ₃ ·2H ₂ O	2.287(3)-2.391(4)	2.497(4)-2.521(5)	3.5233(6)	52.7-64.9	67.81(12)-143.99(13)	16(a)
4-fluorobenzaldehyde Dy(acac) ₃ ·2H ₂ O	2.299(3)-2.443(4)	2.509(5)-2.551(5)	3.5659(6)	52.12-57.52	67.81(12)-143.99(13)	16(b)
Benzaldehyde Dy(acac) ₃ ·2H ₂ O	2.279(4)-2.413(4)	2.516(5)-2.552(5)	3.5391(9)	52.7-64.9	67.25(14)-146.55(14)	16(c)

Table S7. The Dy^{III} geometry analysis by SHAPE 2.0 for complex **3**.

	Square antiprism (D_{4d})	Triangular dodecahedron (D_{2d})	Biaugmented trigonal prism J50 (C_{2v})	Biaugmented trigonal prism (C_{2v})	Snub diphenoid J84 (D_{2d})
Dy1	0.950	2.385	2.271	1.677	4.502
Dy2	1.462	2.064	2.812	2.018	4.966

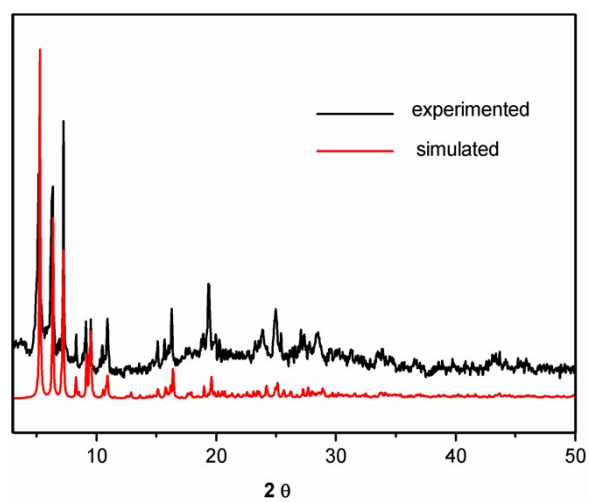


Fig. S1 PXRD pattern of complex 1.

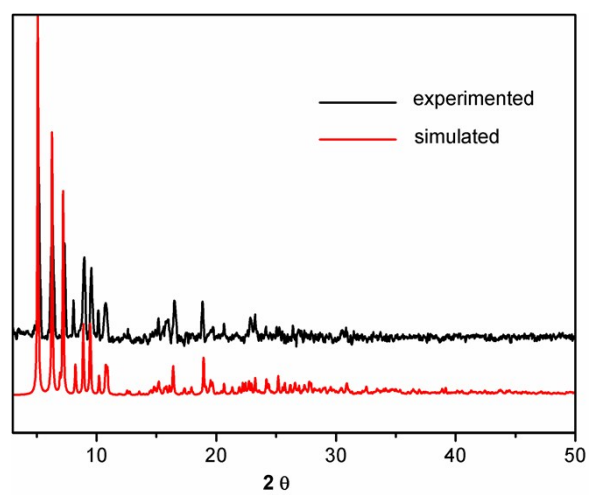


Fig. S2 PXRD pattern of complex 2.

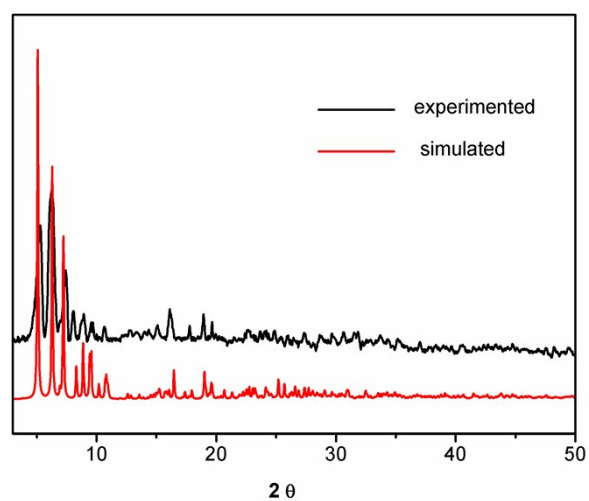


Fig. S3 PXRD pattern of complex 3.

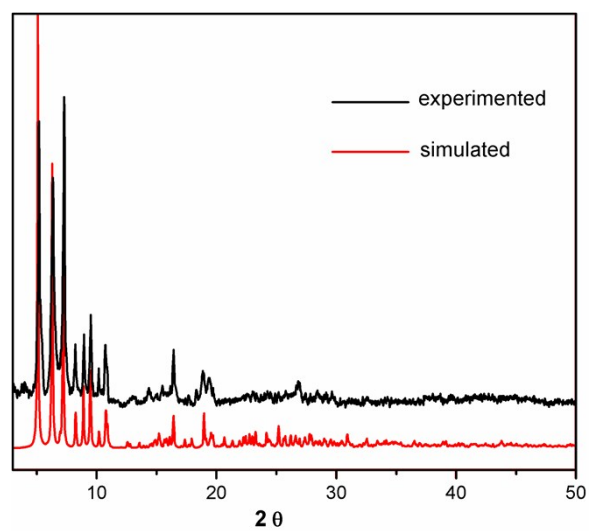


Fig. S4 PXRD pattern of complex 4.

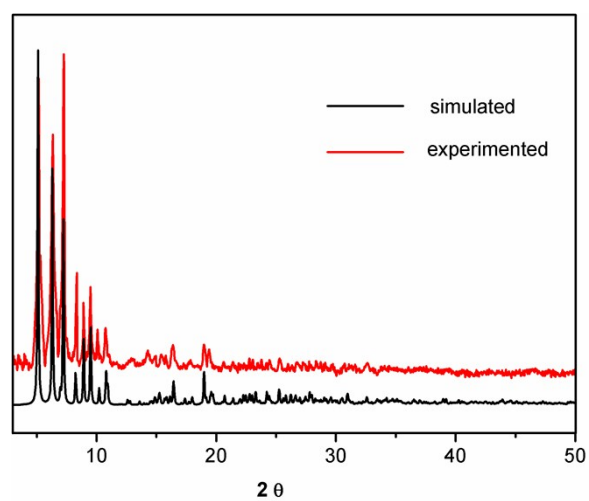


Fig. S5 PXRD pattern of complex 5.

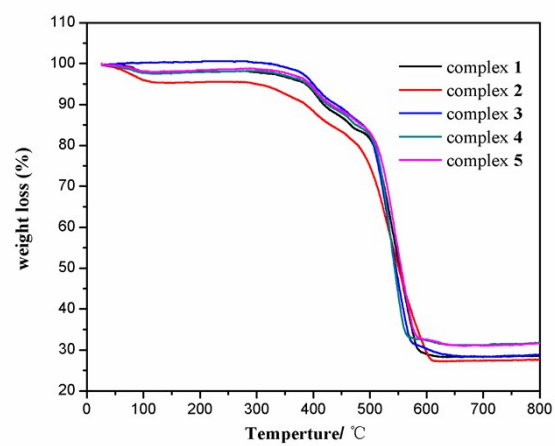


Fig. S6 TGA spectra of complexes 1-5.

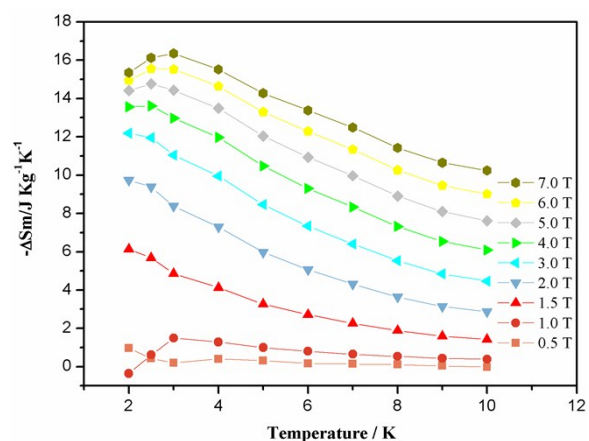


Fig. S7 Temperature dependencies of magnetic entropy change ($-\Delta S_m$) as calculated from the magnetization data of **1** at $T = 2$ -10 K and 0-7 T.

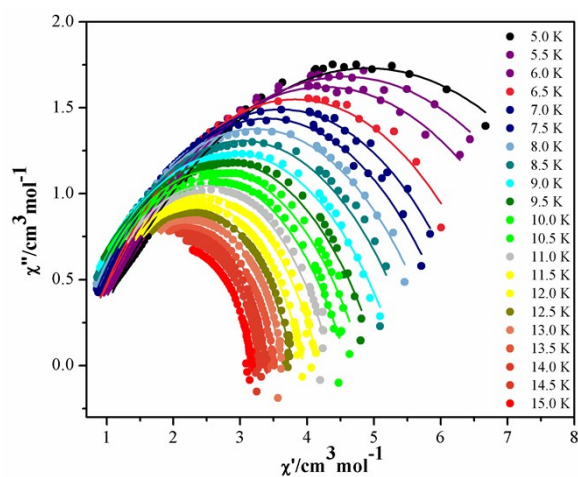


Fig. S8 Cole–Cole plots measured at 2–14 K for **3** ($H_{dc} = 0$ Oe), the solid lines are the best fits to the experimental data, obtained with the generalized Debye model with $\alpha = 0.21$ –0.51.