

Supporting information for

Highly pH-dependent synthesis of two novel three-dimensional dysprosium complexes with interesting magnetic and luminescent properties

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Table S1 Selected bond lengths (Å) and angles (°) for compounds 1–2

Compound 1			
Dy(1)–O(1) ¹	2.396(2)	Dy(2)–O(5)	2.347(2)
Dy(1)–O(2) ¹	2.488(2)	Dy(2)–O(8)	2.320(2)
Dy(1)–O(4)	2.298(2)	Dy(2)–O(11) ²	2.355(2)
Dy(1)–O(7)	2.337(2)	Dy(2)–O(13) ³	2.432(2)
Dy(1)–O(10) ²	2.286(2)	Dy(2)–O(14) ³	2.476(2)
Dy(1)–O(17)	2.344(3)	Dy(2)–O(16)	2.314(2)
Dy(1)–O(20W)	2.449(2)	Dy(2)–O(19)	2.347(3)
Dy(1)–O(21W)	2.420(3)	Dy(2)–O(22W)	2.476(3)
O(1) ¹ –Dy(1)–O(2) ¹	53.35(8)	O(14) ³ –Dy(2)–O(22)	115.14(9)
O(1) ¹ –Dy(1)–O(20)	75.89(8)	O(5)–Dy(2)–O(13) ³	82.54(9)
O(1) ¹ –Dy(1)–O(21)	84.58(9)	O(5)–Dy(2)–O(14) ³	71.31(8)
O(4)–Dy(1)–O(1) ¹	144.98(9)	O(5)–Dy(2)–O(19)	140.13(9)
O(4)–Dy(1)–O(2) ¹	141.99(8)	O(5)–Dy(2)–O(22)	140.66(9)
O(4)–Dy(1)–O(7)	80.88(9)	O(8)–Dy(2)–O(5)	76.50(9)
O(4)–Dy(1)–O(17)	128.59(9)	O(8)–Dy(2)–O(13) ³	130.98(8)
O(4)–Dy(1)–O(20)	69.86(9)	O(8)–Dy(2)–O(14) ³	78.40(8)

O(4)–Dy(1)–O(21)	77.72(9)	O(8)–Dy(2)–O(19)	80.02(9)
Compound 2			
Dy(1)–O(2)	2.364(3)	Dy(2)–O(1)	2.324(3)
Dy(1)–O(4) ¹	2.343(3)	Dy(2)–O(4) ¹	2.676(3)
Dy(1)–O(7)	2.345(3)	Dy(2)–O(5) ¹	2.399(3)
Dy(1)–O(11) ²	2.404(3)	Dy(2)–O(8)	2.334(3)
Dy(1)–O(16) ³	2.454(3)	Dy(2)–O(10) ²	2.269(3)
Dy(1)–O(17) ³	2.427(3)	Dy(2)–O(14)	2.296(3)
Dy(1)–O(19)	2.366(3)	Dy(2)–O(20)	2.325(4)
Dy(1)–O(21W)	2.396(3)	Dy(2)–O(22W)	2.376(3)
O(2)–Dy(1)–O(10) ²	65.86(9)	O(1)–Dy(2)–O(4) ¹	71.51(9)
O(2)–Dy(1)–O(11) ²	78.77(11)	O(1)–Dy(2)–O(5) ¹	83.42(11)
O(2)–Dy(1)–O(16) ³	141.41(10)	O(1)–Dy(2)–O(8)	138.03(10)
O(2)–Dy(1)–O(17) ³	146.37(11)	O(1)–Dy(2)–O(20)	130.43(14)
O(2)–Dy(1)–O(19)	74.74(11)	O(1)–Dy(2)–O(22)	131.89(11)
O(2)–Dy(1)–O(21)	75.25(10)	O(5) ¹ –Dy(2)–O(4) ¹	50.61(10)
O(4) ¹ –Dy(1)–O(2)	77.04(10)	O(8)–Dy(2)–O(4) ¹	70.05(10)
O(4) ¹ –Dy(1)–O(7)	71.00(10)	O(8)–Dy(2)–O(5) ¹	85.09(11)
O(4) ¹ –Dy(1)–O(10) ²	73.79(10)	O(8)–Dy(2)–O(22)	75.60(11)

Symmetry transformations used to generate equivalent atoms in complex **1**: ¹-x, 1/2+y, 1/2-z; ²-1+x, 1/2-y, -1/2+z; ³1-x, -1/2+y, 1/2-z; and complex **2**: ¹-1/2+x, 3/2-y, +z; ²1/2+x, 1/2-y, +z; ³1/2-x, -1/2+y, 1/2+z.

Table S2 Continuous Shape Measures (CSHM's) calculated by SHAPE 2.1 for **1** and **2**.^a

	1-Dy1	1-Dy2	2-Dy1	2-Dy2
OP-8	31.304	30.455	31.047	31.707
HPY-8	22.404	22.498	22.764	21.692
HBPY-8	15.246	15.656	14.006	15.347
CU-8	10.908	11.462	9.621	10.629
SAPR-8	2.557	1.812	2.795	3.64
TDD-8	1.48	1.851	2.081	1.955
JGBF-8	12.769	14.166	12.763	12.645
JETBPY-8	28.367	27.771	24.555	24.536
JBTPR-8	2.15	1.887	2.661	3.229
BTPR-8	1.565	1.133	1.732	2.89
JSD-8	3.65	3.881	4.641	3.87
TT-8	11.73	11.947	10.453	11.152
ETBPY-8	24.044	22.543	19.871	21.495

^a List Of Reference Shapes:

OP-8	D8h	Octagon
HPY-8	C7v	Heptagonal pyramid
HBPY-8	D6h	Hexagonal bipyramid

CU-8	Oh	Cube
SAPR-8	D4d	Square antiprism
TDD-8	D2d	Triangular dodecahedron
JGBF-8	D2d	Johnson gyrobifastigium J26
JETBPY-8	D3h	Johnson elongated triangular bipyramid J14
JBTPR-8	C2v	Biaugmented trigonal prism J50
BTPR-8	C2v	Biaugmented trigonal prism
JSD-8	D2d	Snub diphenooid J84
TT-8	Td	Triakis tetrahedron
ETBPY-8	D3h	Elongated trigonal bipyramid

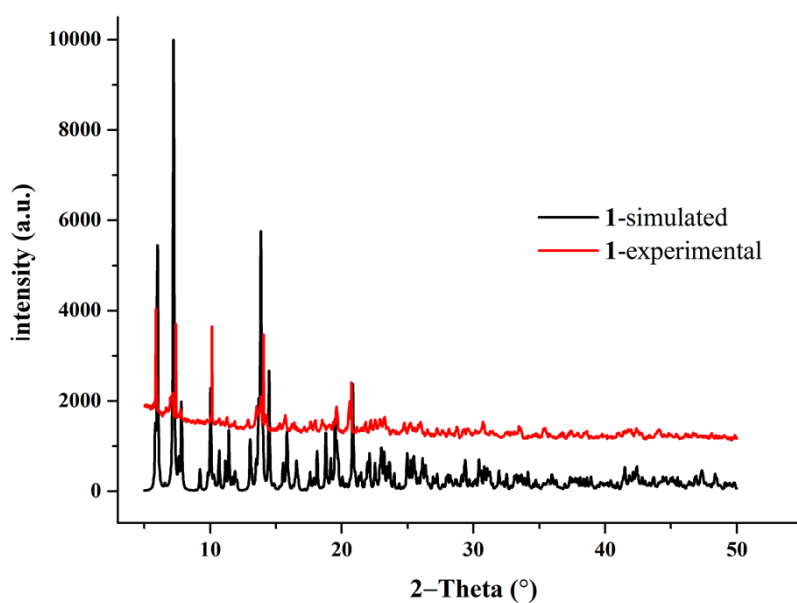


Figure S1. Experimental and simulated PXRD patterns for **1**.

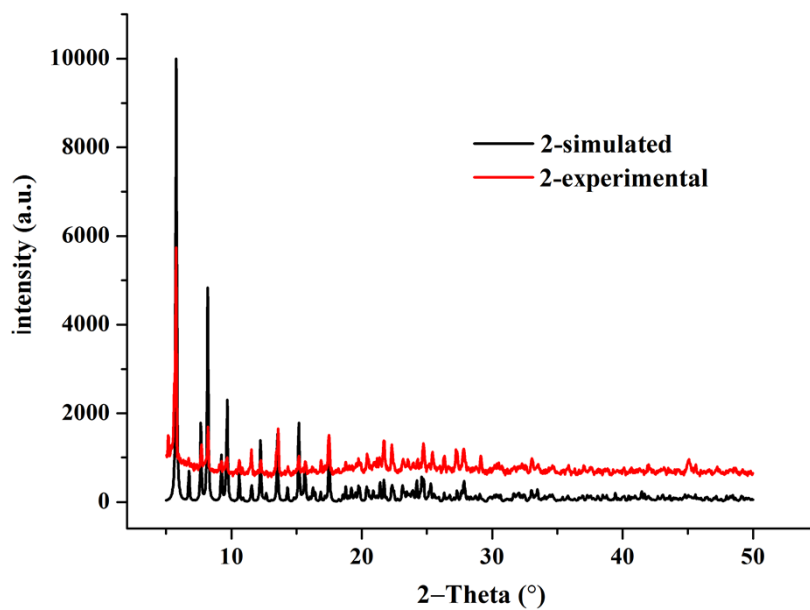


Figure S2. Experimental and simulated PXRD patterns for **2**.

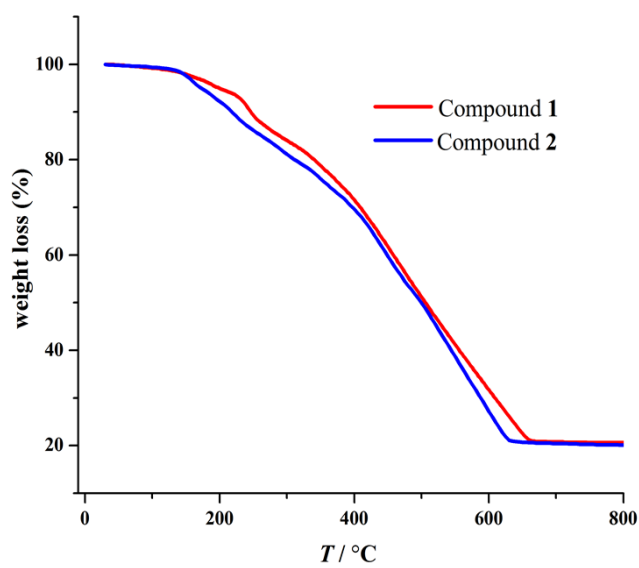


Figure S3. The TGA curves for compound **1** and **2**.

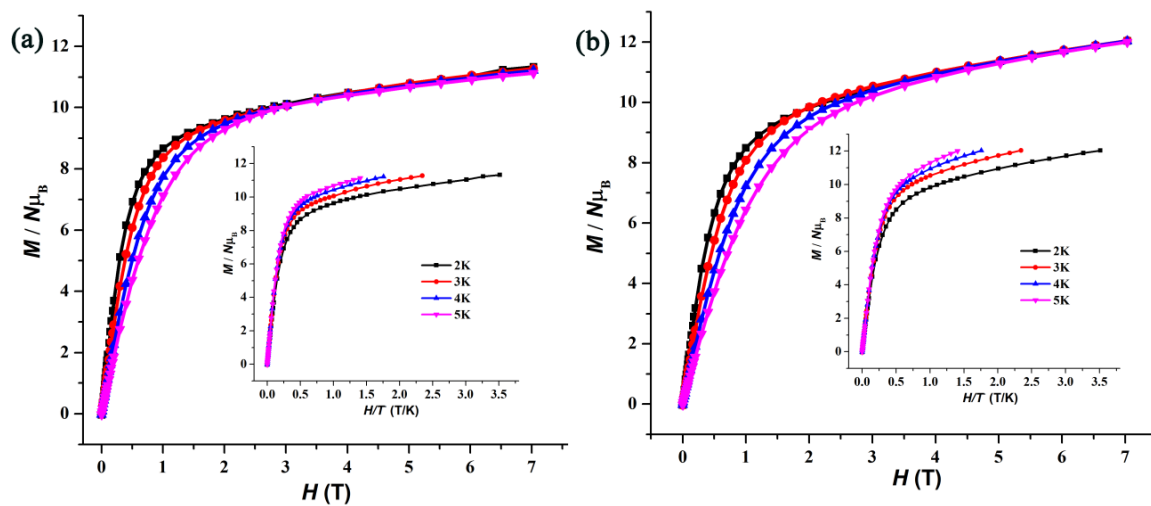


Figure S4. Plots of magnetization (M) vs field (H) for compounds **1** (a) and **2** (b) at different low temperatures. Insets: M vs H/T plots at different temperatures.