Electronic supplementary information

Syntheses, structures and magnetic properties of three dinuclear, one-dimensional and two-dimensional Dysprosium(III) complexes based on naphthalene diimide salicylic acid

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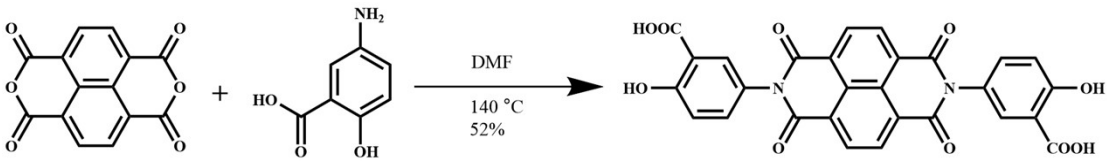

Scheme S1. Synthesis of N,N'-bis(3-carboxy-4-hydroxyphenyl)-1,4,5,8-naphthalenetetradicarboximide (H_4NDISA).

Table S1. geometry analysis by using SHAPE 2.0 program (complex **1** and **3**)

	SAPR-8 (D_{4d})	TDD-8 (D_{2h})	JBTPR-8 (C_{2V})	BTPR-8 (C_{2v})	JSD-8 (D_{2d})
1	**1.0003**	**0.9829**	**1.8019**	**1.4860**	**2.8753**
3	**3.7518**	**1.1756**	**4.0640**	**3.6774**	**4.4688**

Table S2. geometry analysis by using SHAPE 2.0 program (complex **2**)

	JCSAPR-9 (C_{4V})	CSAPR-9 (C_{4v})	JTCTPR-9 (D_{3h})	TCTPR-9 (D_{3h})	MFF-9 (C_S)
2	**1.9197**	**0.8247**	**2.6546**	**1.1809**	**1.2309**

*SAPR-8 = Square antiprism; TDD-8 = Triangular dodecahedron;
JBTPR-8 = Biaugmented trigonal prism; BTPR-8 = Biaugmented trigonal prism;
JSD-8 = Snub diphenoid; JCSAPR-9 = Capped square antiprism;
CSAPR-9 = Spherical capped square antiprism; JTCTPR-9 = Tricapped trigonal prism;
TCTPR-9 = Spherical tricapped trigonal prism; MFF-9 = Muffin.

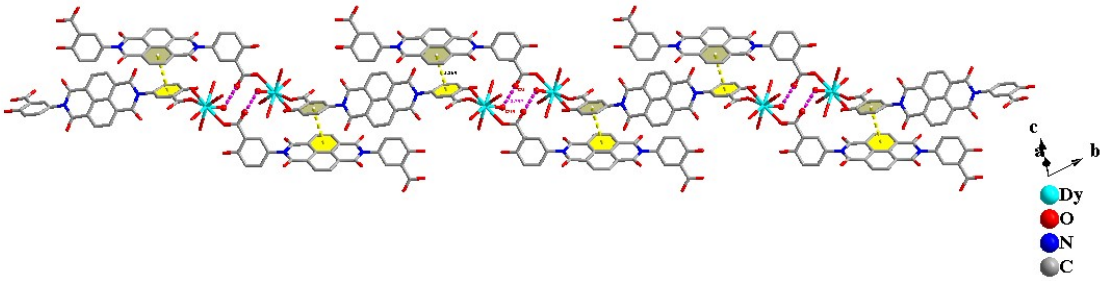

Figure S1. For **1**, inter-molecular O19-H19B···O3 hydrogen bonding interaction and 1D face-to-face π-π stacking interaction. Hydrogen atoms and part solvent molecules were omitted for clarity. Color code: Dy, green; O, red; N, blue; C, gray. Hydrogen atoms and uncoordinated solvent molecules were omitted for clarity.

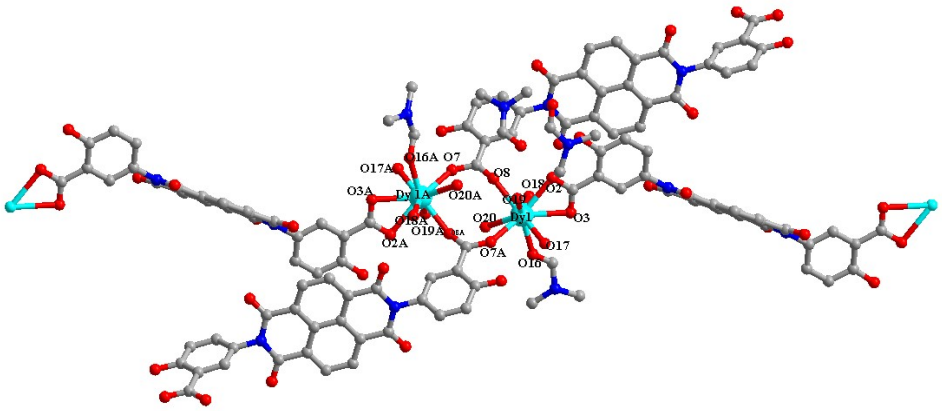

Figure S2. For **2**, crystal structure. Hydrogen atoms and part solvent molecules were omitted for clarity. Color code: Dy, green; O, red; N, blue; C, gray. Hydrogen atoms and uncoordinated solvent molecules were omitted for clarity.

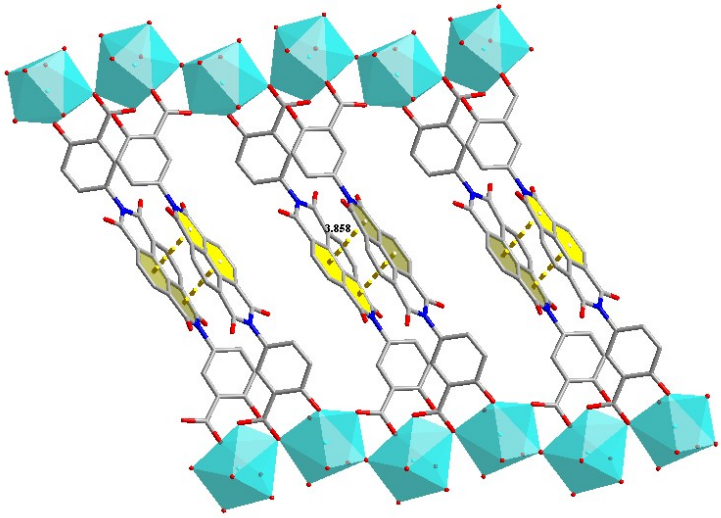

Figure S3. For **3**, 1D face-to-face π-π stacking interaction. Hydrogen atoms and part solvent molecules were omitted for clarity. Color code: Dy, green; O, red; N, blue; C, gray. Hydrogen atoms and uncoordinated solvent molecules were omitted for clarity.

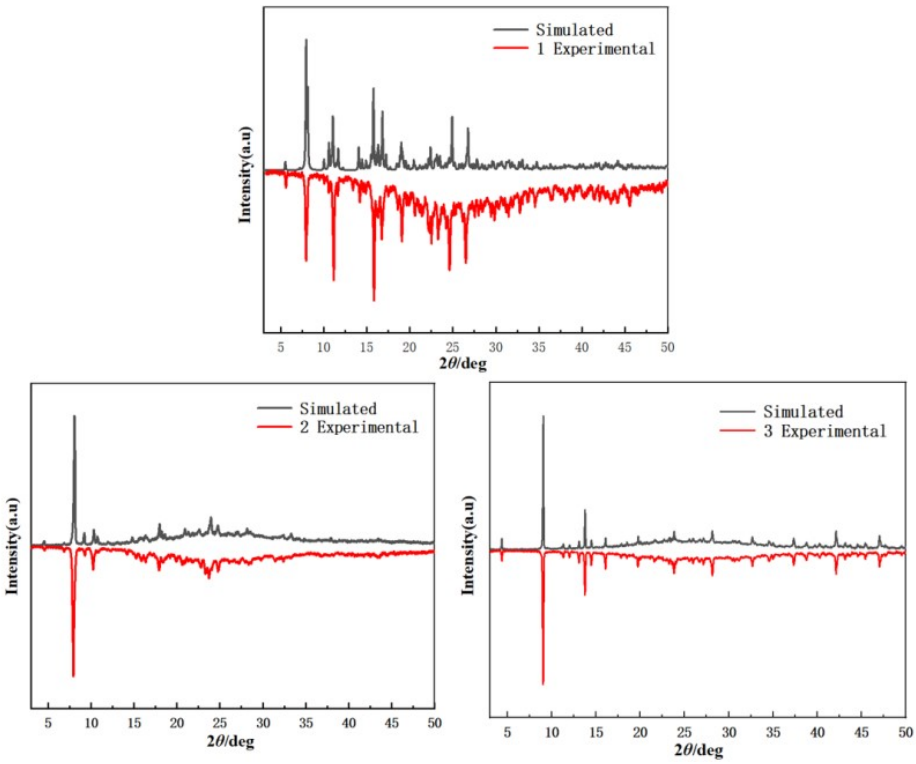

Figure S4. Powder X-ray diffraction (PXRD) patterns for complexes **1-3**.

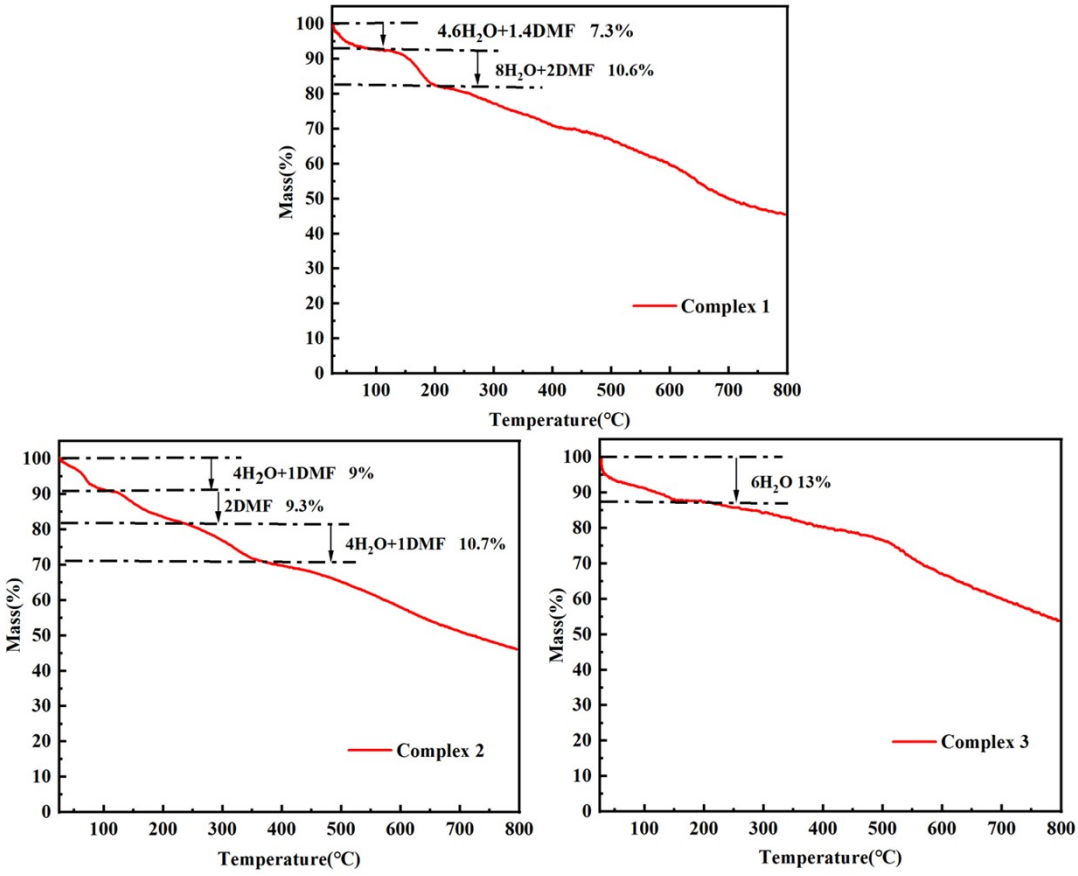

Figure S5 TG curves of complexes **1-3**.

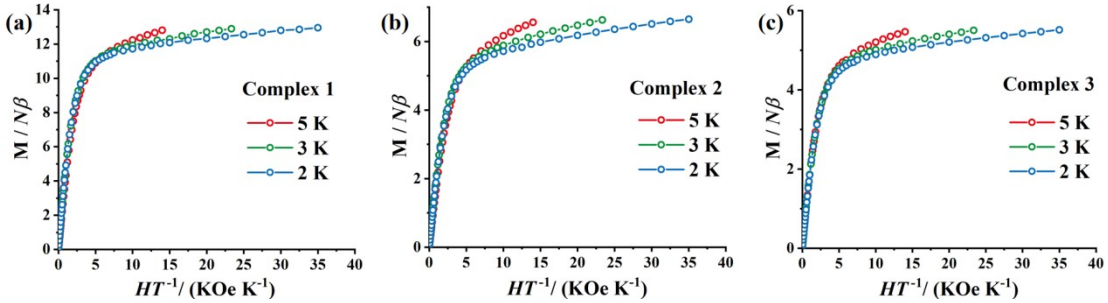

Figure S6. M versus H/T curves for **1**-**3** (a-c).

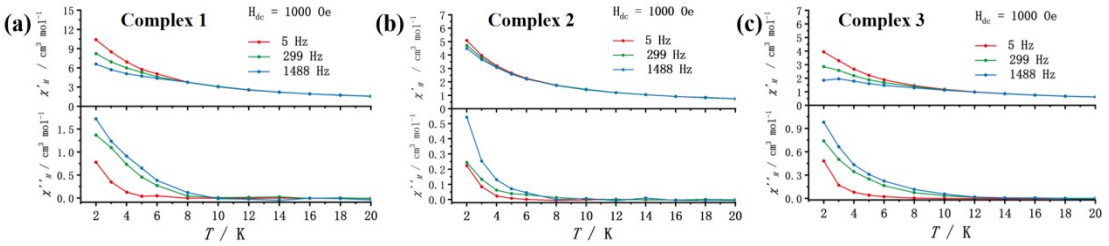

Figure S7. Temperature dependence of χ'_M product and χ''_M for complexes **1**-**3** (a-c) in a 1000 Oe dc field.

Table S3. Crystallographic data and redefinement parameters for complex **1-3**

Identification code	**1**	**2**	**3**
Empirical formula	$C_{96}H_{88}Dy_2N_{10}O_{46}$	$C_{54}H_{58}DyN_7O_{25}$	$C_{28}H_{19}DyN_2O_{14}$
Formula weight	2442.76	1367.57	769.95
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/n$
a/Å	11.7197(2)	11.5540(2)	8.8770(3)
b/Å	12.7121(2)	12.8863(2)	37.7347(9)
c/Å	17.4599(3)	19.4414(3)	8.9024(4)
α/°	74.413(2)	83.0210(10)	90
β/°	71.436(2)	74.564(2)	119.789(5)
γ/°	86.5400(10)	84.6300(10)	90
Volume/Å^3	2374.28(8)	2763.83(8)	2587.99(19)
Z	1	2	4
ρ_{calc}g/cm^3	1.708	1.643	1.976
μ/mm^{-1}	1.670	8.062	2.972
F(000)	1234.0	1394.0	1516.0
Reflections collected	35944	40597	34502
Independent reflections	12043	10870	5955
Data/restraints/parameters	12043/46/793	10870/36/830	5955/0/407
Goodness-of-fit on F^2	1.072	1.054	1.124
Final R indexes [I>=2σ (I)]	R_1 = 0.0398, wR_2 = 0.1018	R_1 = 0.0514, wR_2 = 0.1348	R_1 = 0.0382, wR_2 = 0.0738
Final R indexes [all data]	R_1 = 0.0489, wR_2 = 0.1059	R_1 = 0.0588, wR_2 = 0.1396	R_1 = 0.0483, wR_2 = 0.0768
Largest diff. peak/hole/ e Å^{-3}	2.00/-1.16	1.32/-1.11	1.24/-1.92
CCDC	2369945	2369946	2369947

Table S4. Selected bond lengths (Å) and angles (°) for complex **1**

Complex **1**			
Dy1-O16	2.290(3)	O16-Dy1-O2	80.80(10)
Dy1-O22	2.30(4)	O22-Dy1-O2	71.6(10)
Dy1-O12	2.320(2)	O12-Dy1-O2	144.85(9)
Dy1-O21	2.335(13)	O21-Dy1-O2	71.6(4)
Dy1-O19	2.347(2)	O19-Dy1-O2	74.73(9)
Dy1-O2	2.398(2)	O16-Dy1-O18	145.11(11)
Dy1-O18	2.411(3)	O22-Dy1-O18	69.9(9)
Dy1-O20	2.417(3)	O12-Dy1-O18	73.04(9)
Dy1-O17	2.423(3)	O21-Dy1-O18	78.2(3)
O16-Dy1-O22	96.6(8)	O19-Dy1-O18	69.09(9)
O16-Dy1-O12	104.83(10)	O2-Dy1-O18	121.57(8)
O22-Dy1-O12	139.6(10)	O16-Dy1-O20	73.39(10)
O16-Dy1-O21	85.6(3)	O22-Dy1-O20	144.0(10)
O12-Dy1-O21	142.6(4)	O12-Dy1-O20	75.81(9)
O16-Dy1-O19	145.79(10)	O21-Dy1-O20	140.9(4)
O22-Dy1-O19	97.9(8)	O19-Dy1-O20	76.70(9)
O12-Dy1-O19	83.24(9)	O2-Dy1-O20	72.71(9)
O21-Dy1-O19	108.3(3)	O18-Dy1-O20	135.70(10)
O16-Dy1-O17	73.52(12)	O19-Dy1-O17	140.18(11)
O22-Dy1-O17	76.4(9)	O2-Dy1-O17	135.89(11)
O12-Dy1-O17	77.44(11)	O18-Dy1-O17	72.06(11)
O21-Dy1-O17	71.2(4)	O20-Dy1-O17	129.77(11)

Table S5. Selected bond lengths (Å) and angles (°) for complex **2**

Complex-**2**			
Dy1-O7[1]	2.410(3)	O7[1]-Dy1-O3	140.91(10)
Dy1-O2	2.475(3)	O7[1]-Dy1-O20	68.74(10)
Dy1-O3	2.536(3)	O7[1]-Dy1-O18	139.55(11)
Dy1-O8	2.358(3)	O7[1]-Dy1-C7	149.29(11)
Dy1-O20	2.430(3)	O2-Dy1-O3	51.94(10)
Dy1-O19	2.408(3)	O2-Dy1-C7	26.39(12)
Dy1-O18	2.417(3)	O3-Dy1-C7	25.56(12)
Dy1-O17	2.405(3)	O8-Dy1-O7[1]	93.04(10)
Dy1-O16	2.353(3)	O8-Dy1-O2	77.64(10)
O7[1]-Dy1-O2	141.08(11)	O8-Dy1-O3	123.93(10)
O16--Dy1-O17	71.18(12)	O16-Dy1-C7	98.93(12)
O16-Dy1-O18	82.14(12)	O16-Dy1-O19	139.52(12)
O16-Dy1O20	71.74(11)	O16-Dy1-O3	73.42(11)
O16-Dy1-O8	142.99(11)	O16-Dy1-O2	125.15(11)
O16-Dy1-O7[1]	84.37(11)	O17-Dy1-C7	81.47(12)
O17-Dy1-O18	137.75(11)	O17-Dy1-O3	71.87(11)
O17--Dy1-O19	70.40(12)	O17-Dy1-O2	93.72(11)
O17-Dy1-O20	126.62(11)	O17-Dy1-O7[1]	70.65(11)
O18-Dy1-C7	70.79(12)	O18-Dy1-O20	70.82(10)
O18-Dy1-O2	75.30(11)	O18-Dy1-O3	69.40(11)
O8-Dy1-O20	72.97(11)	O8-Dy1-O19	72.05(11)
O19-Dy1-C7	87.59(12)	O19-Dy1-O3	105.78(10)
O19-Dy1-O18	136.68(11)	O19-Dy1-O2	69.81(10)
O19-Dy1-O20	124.31(10)	O19-Dy1-O7[1]	71.37(10)
O20-Dy1-C7	141.38(11)	O20-Dy1-O3	129.66(10)
O20-Dy1-O2	139.31(11)	O8-Dy1-C7	101.64(12)
O8-Dy1-O17	142.15(11)	O8-Dy1-O18	76.13(11)

Table S6. Selected bond lengths (Å) and angles (°) for complex **3**

Complex **3**			
Dy1-O1	2.239(3)	O1-Dy1-O2	71.95(10)
Dy1-O9^{2}	2.354(3)	O1-Dy1-O3^{1}	83.09(11)
Dy1-O10^{3}	2.318(3)	O1-Dy1-O9^{2}	139.18(10)
Dy1-O11	2.361(3)	O1-Dy1-O10^{3}	76.80(11)
Dy1-O12	2.384(3)	O1-Dy1-O11	92.96(11)
Dy1-O2^{1}	2.541(3)	O1-Dy1-O12	152.89(11)
Dy1-O2	2.428(3)	O1-Dy1-C7^{1}	89.86(11)
Dy1-O3^{1}	2.416(3)	O2-Dy1-O2^{1}	139.42(9)
O1-Dy1-O2^{1}	95.83(10)	O2-Dy1-C7^{1}	113.03(11)
O12-Dy1-C7^{1}	95.99(11)	O11-Dy1-O2^{1}	145.40(10)
O12-Dy1-O3^{1}	112.59(11)	O11-Dy1-O2	75.01(10)
O12-Dy1-O2^{1}	78.90(10)	O10^{3}-Dy1-C7^{1}	100.30(11)
O12-Dy1-O2	128.35(10)	O10^{3}-Dy1-O12	76.11(11)
O11-Dy1-C7^{1}	171.96(11)	O10^{3}-Dy1-O11	73.08(11)
O11-Dy1-O12	78.16(11)	O10^{3}-Dy1-O9^{2}	143.96(10)
O11-Dy1-O3^{1}	162.33(10)	O10^{3}-Dy1-O3^{1}	122.21(11)
O9^{2}-Dy1-C7^{1}	81.54(11)	O10^{3}-Dy1-O2^{1}	76.50(10)
O9^{2}-Dy1-O12	67.93(10)	O10^{3}-Dy1-O2	133.46(10)
O9^{2}-Dy1-O11	101.05(11)	O9^{2}-Dy1-O3^{1}	72.04(11)
O3^{1}-Dy1-C7^{1}	25.67(11)	O9^{2}-Dy1-O2	75.01(10)
O3^{1}-Dy1-O2	87.41(10)	O9^{2}-Dy1-O2^{1}	93.87(10)
O3^{1}-Dy1-O2^{1}	52.27(9)	O21-Dy1-C7^{1}	26.62(10)