Supporting information for

From 1D to 3D: dimensional control of low-coordinate lanthanide coordination polymers with SMM feature and white-light emission

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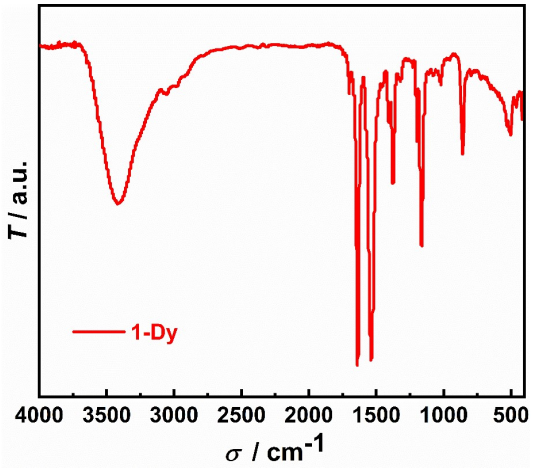
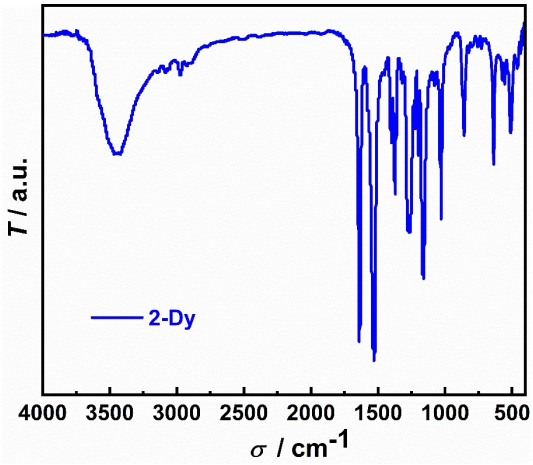
Table S1 Crystallographic data and structure refinement for complexes **1-3**.

	1-Dy	**2-Dy**	**3-Dy**
Formula	$C_{57}H_{76}C_{l3}DyN_6O_{15}$	$C_{57}H_{58}DyF_9N_6O_{17}S_3$	$C_{57}H_{60}DyF_9N_6O_{18}S_3$
M_r (g mol^{-1})	1354.08	1528.77	1546.79
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1$	P-1	C2/c
T (K)	173	196	173
a (Å)	14.3586(3)	10.1389(11)	20.8029(12)
b (Å)	13.8397(3)	13.1621(14)	20.6147(14)
c (Å)	15.6337(4)	14.2513(15)	17.7986(11)
α (º)	90	74.195(2)	90
β (º)	90.7110(10)	73.041(2)	116.797(2)

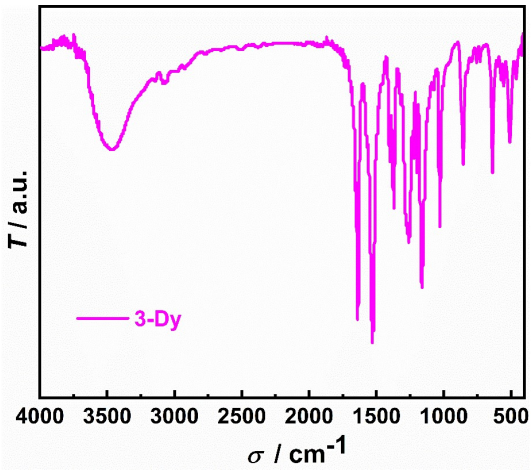
γ (°)	90	77.071(2)	90
V (Å^3)	3106.47(12)	1728.7(3)	6813.2(7)
Z	2	1	4
D_c (g cm^{-3})	1.448	1.468	1.508
μ (mm^{-1})	1.400	1.262	1.283
F(000)	1394.0	773.0	3132.0
Reflns collected	40714	9556	19333
Unique reflns	12580	5949	6214
R_{int}	0.022(9)	0.0297	0.0664
GOF	1.038	1.076	1.083
R_1(I > 2σ)	0.0324	0.0583	0.0826
wR_2 (all data)	0.0772	0.1984	0.2411
Max. diff. peak / hole (e Å^{-3})	1.22/-0.53	1.55/-1.43	1.93/-1.71



(a)

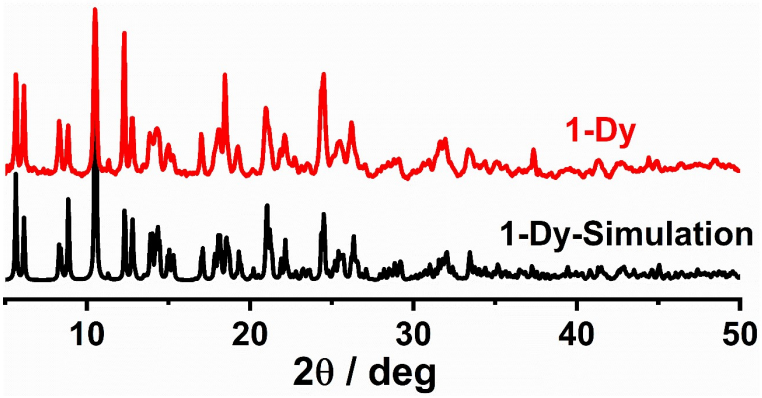


(b)

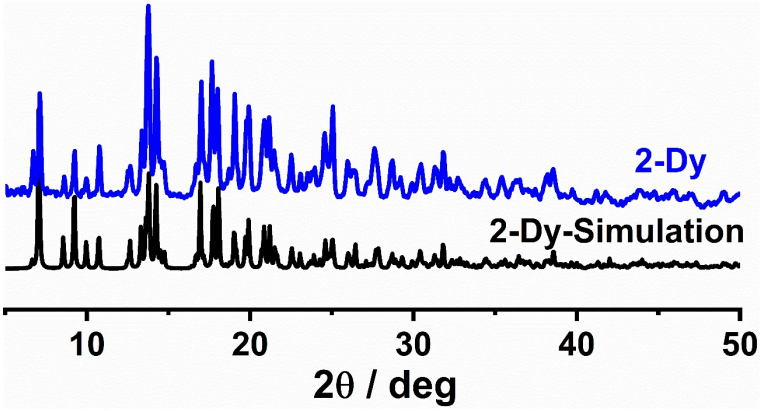


(c)

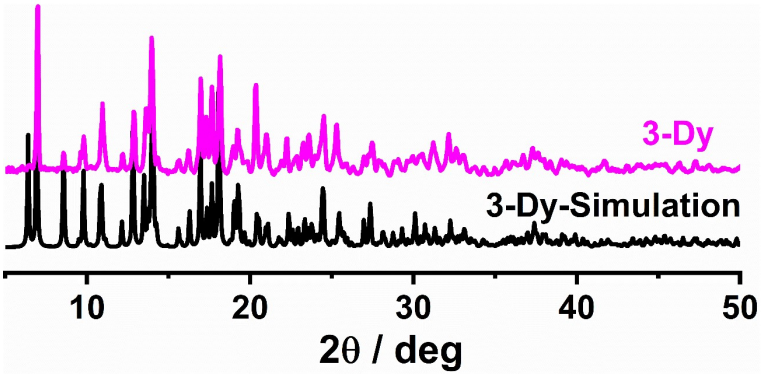
Fig. S1 IR spectra of complexes **1**-**3** (a-c).



(a)



(b)



(c)

Fig. S2 Measured and simulated PXRD patterns of complexes **1-3**.

Table S2 Continuous shape measures (CShM) for complexes **1-3**.

	1-Dy	**3-Dy**		**2-Dy**
HP-7	35.493	28.352	HP-6	32.656
HPY-7	19.836	24.203	PPY-6	30.061
PBPY-7	5.341	**4.069**	OC-6	**0.014**
COC-7	**1.188**	7.695	TPR-6	16.478
CTPR-7	**0.877**	6.666	JPPY-6	33.574

JPBPY-7	8.381	7.961
JETPY-7	20.918	18.279

HP-7 = Heptagon, HPY-7 = Hexagonal pyramid, **PBPY-7 = Pentagonal bipyramid**, **COC-7** = **Capped octahedron**, **CTPR-7 = Capped trigonal prism**, JPBPY-7 = Johnson pentagonal bipyramid J13, JETPY-7 = Johnson elongated triangular pyramid J7

HP-6 = Hexagon, PPY-6 = Pentagonal pyramid, **OC-6 = Octahedron**, TPR-6 = Trigonal prism, JPPY-6 = Johnson pentagonal pyramid J2

Table S3 Selected bond lengths (Å) and angles (º) for **1**-**3**.

1		**2**		**3**	
Dy(1)-O(1)	2.349(5)	Dy(1)-O(1)	2.254(5)	Dy(1)-O(1)	2.210(14)
Dy(1)-O(2)#1	2.248(4)	Dy(1)-O(1)#3	2.254(5)	Dy(1)-O(1)#8	2.210(14)
Dy(1)-O(3)#2	2.310(5)	Dy(1)-O(2)#4	2.246(5)	Dy(1)-O(2)#6	2.260(6)
Dy(1)-O(4)	2.249(4)	Dy(1)-O(2)#5	2.246(5)	Dy(1)-O(2)#9	2.260(6)
Dy(1)-O(5)#1	2.361(5)	Dy(1)-O(3)#6	2.242(5)	Dy(1)-O(3)#10	2.285(6)
Dy(1)-O(6)#2	2.289(5)	Dy(1)-O(3)#7	2.242(5)	Dy(1)-O(3)#11	2.285(6)
Dy(1)-O(7)	2.356(4)	O(1)#3-Dy(1)-O(1)	180	Dy(1)-O(4)	2.426(16)
O(1)-Dy(1)-O(5)#1	153.28(18)	O(2)#4-Dy(1)-O(1)#3	90.5(2)	O(1)-Dy(1)-O(1)#8	122.1(9)
O(1)-Dy(1)-O(7)	76.7(3)	O(2)#4-Dy(1)-O(1)	89.5(2)	O(1)#8-Dy(1)-O(2)#6	91.3(4)
O(2)#1-Dy(1)-O(1)	101.58(17)	O(2)#5-Dy(1)-O(1)	90.5(2)	O(1)-Dy(1)-O(2)#6	87.4(4)
O(2)#1-Dy(1)-O(3)#2	115.18(17)	O(2)#5-Dy(1)-O(1)#3	89.5(2)	O(1)#8-Dy(1)-O(2)#9	87.4(4)
O(2)#1-Dy(1)-O(4)	158.06(16)	O(2)#4-Dy(1)-O(2)#5	180	O(1)-Dy(1)-O(2)#9	91.3(4)
O(2)#1-Dy(1)-O(5)#1	76.67(17)	O(3)#6-Dy(1)-O(1)	91.6(2)	O(1)-Dy(1)-O(3)#10	157.2(5)
O(2)#1-Dy(1)-O(6)#2	79.06(18)	O(3)#7-Dy(1)-O(1)	88.4(2)	O(1)-Dy(1)-O(3)#11	80.3(4)
O(2)#1-Dy(1)-O(7)	77.74(16)	O(3)#6-Dy(1)-O(1)#3	88.4(2)	O(1)#8-Dy(1)-O(3)#11	157.2(5)
O(3)#2-Dy(1)-O(1)	125.4(2)	O(3)#7-Dy(1)-O(1)#3	91.6(2)	O(1)#8-Dy(1)-O(3)#10	80.3(4)
O(3)#2-Dy(1)-O(5)#1	77.2(2)	O(3)#6-Dy(1)-O(2)#5	89.80(19)	O(1)-Dy(1)-O(4)	61.1(4)
O(3)#2-Dy(1)-O(7)	147.1(2)	O(3)#6-Dy(1)-O(2)#4	90.20(19)	O(1)#8-Dy(1)-O(4)	61.1(4)
O(4)-Dy(1)-O(1)	76.21(17)	O(3)#7-Dy(1)-O(2)#5	90.20(19)	O(2)#9-Dy(1)-O(2)#6	177.3(3)
O(4)-Dy(1)-O(3)#2	82.12(17)	O(3)#7-Dy(1)-O(2)#4	89.80(19)	O(2)#6-Dy(1)-O(3)#11	93.7(2)
O(4)-Dy(1)-O(5)#1	95.44(17)	O(3)#7-Dy(1)-O(3)#6	180	O(2)#9-Dy(1)-O(3)#10	93.7(2)
O(4)-Dy(1)-O(6)#2	120.40(18)			O(2)#9-Dy(1)-O(3)#11	88.4(2)
O(4)-Dy(1)-O(7)	80.54(16)			O(2)#6-Dy(1)-O(3)#10	88.4(2)
O(6)#2-Dy(1)-O(1)	75.2(2)			O(2)#9-Dy(1)-O(4)	88.64(14)
O(6)#2-Dy(1)-O(3)#2	74.0(2)			O(2)#6-Dy(1)-O(4)	88.64(14)
O(6)#2-Dy(1)-O(5)#1	129.2(2)			O(3)#10-Dy(1)-O3#11	77.6(4)
O(6)#2-Dy(1)-O(7)	138.8(2)			O(3)#10-Dy(1)-O(4)	141.19(18)
O(7)-Dy(1)-O5#1	76.9(3)			O(3)#11-Dy(1)-O(4)	141.19(18)

Symmetry codes: #1 +x, -1+y, +z; #2 2-x, -1/2+y, 1-z; #3 1-x, -y, 2-z; #4 -1+x, +y, 1+z; #5 2-x, -y, 1-z; #6 1-x, 1-y, 1-z; #7 +x, -1+y, 1+z; #8 1-x, +y, 3/2-z; #9 +x, 1-y, 1/2+z; #10 -1/2+x, 1/2-y, 1/2+z; #11 3/2-x, 1/2-y, 1-z.

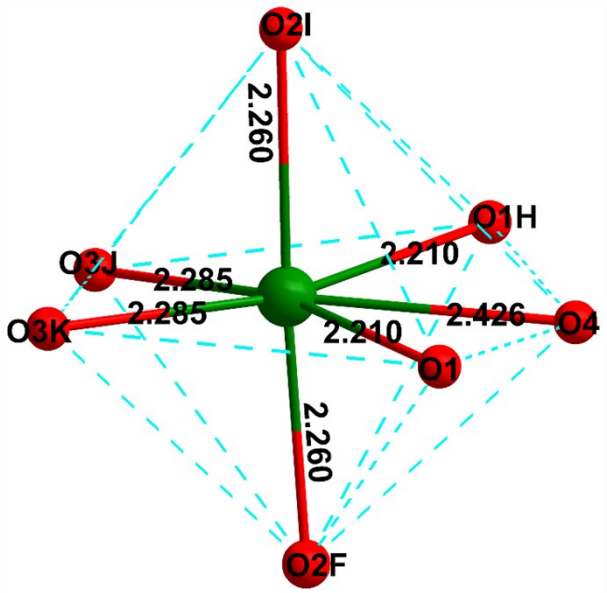
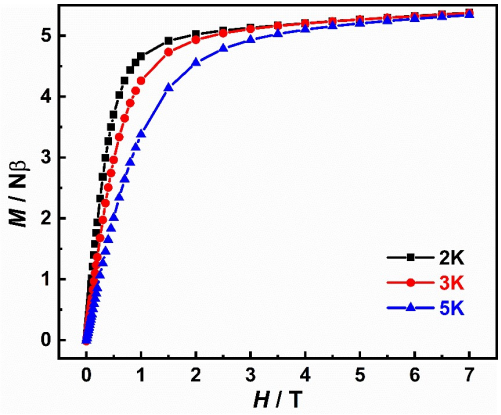
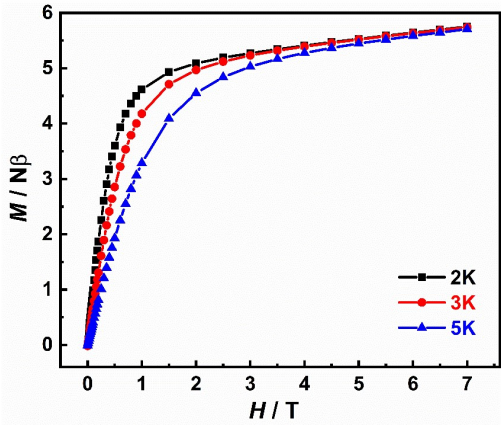


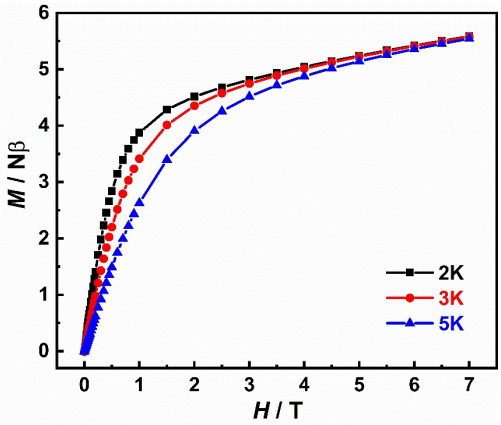
Fig. S3 Pentagonal bipyramidal coordination geometry of Dy(III) in **1**. Dy and O are shown in green and red, respectively. Symmetry codes: F 1-x, 1-y, 1-z; H 1-x, +y, 3/2-z; I +x, 1-y, 1/2+z; J -1/2+x, 1/2-y, 1/2+z; K 3/2-x, 1/2-y, 1-z.



(a)

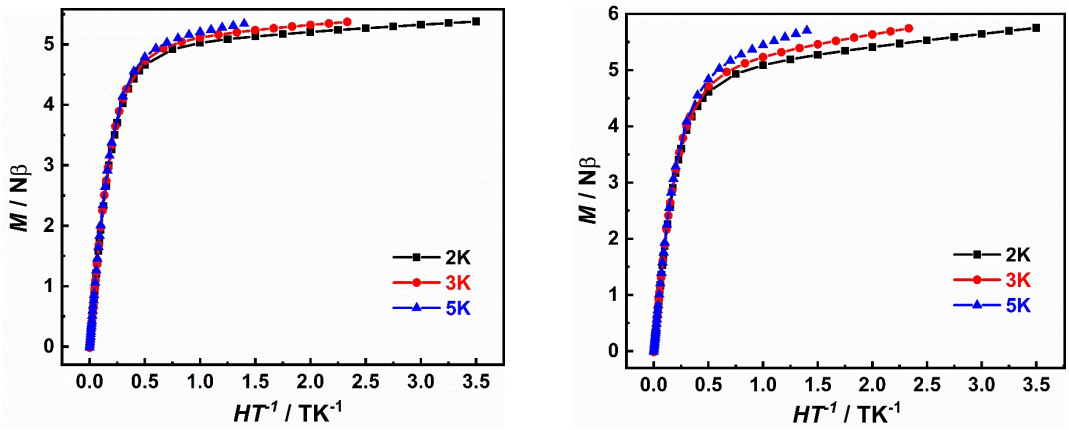


(b)

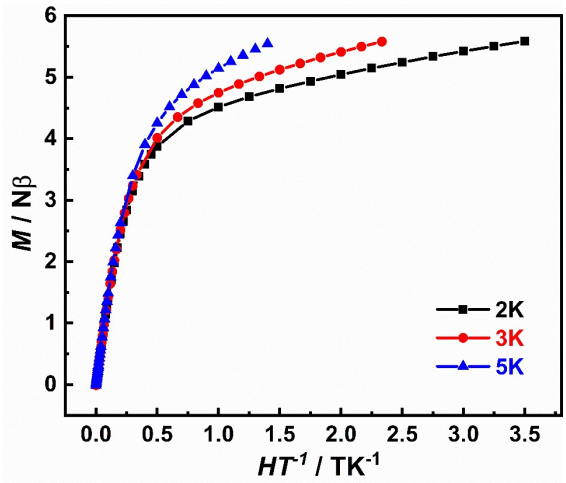


(c)

Fig. S4 *M* vs. *H* plots for **1-3** (a-c).

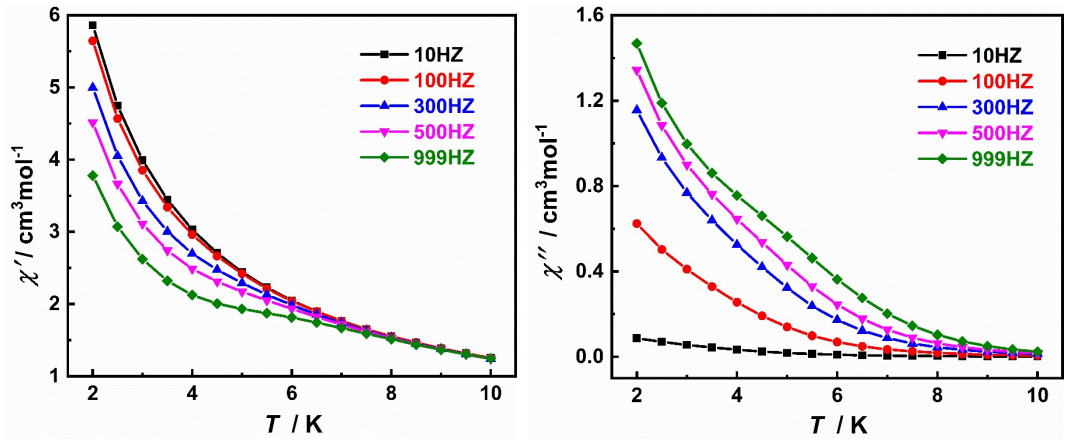


(a) (b)



(c)

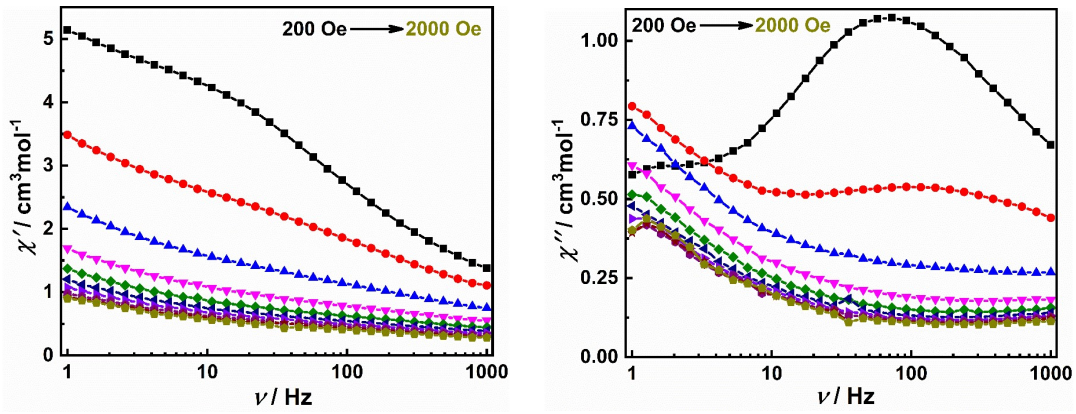
Fig. S5 *M* vs. HT^{-1} plots for **1-3** (a-c).



(a) (b)

Fig. S6 Temperature dependence of in-phase (a) and out-of-phase (b)

AC susceptibility data at a zero DC field for **1**.



(a) (b)

Fig. S7 Frequency dependence of in-phase (a) and out-of-phase (b) AC susceptibility signals under different DC fields at 2 K for **1**.

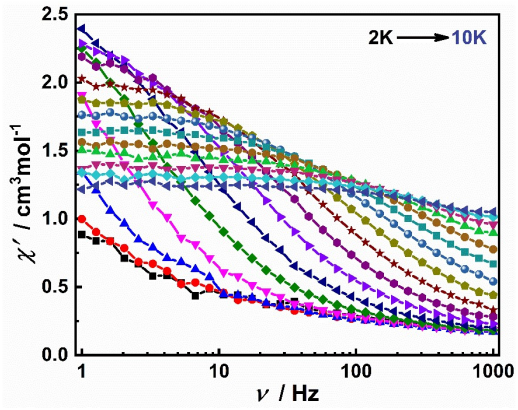
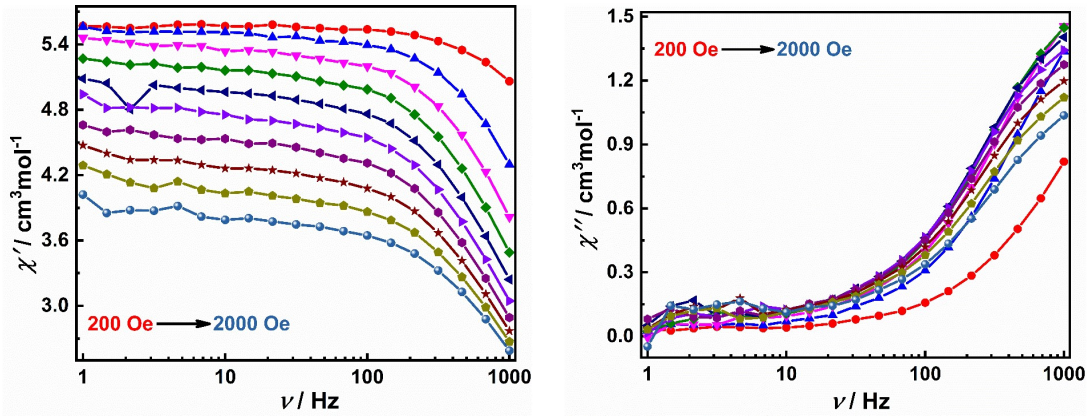


Fig. S8 Frequency dependence of in-phase AC susceptibility data at a 1400 Oe DC field for **1**.

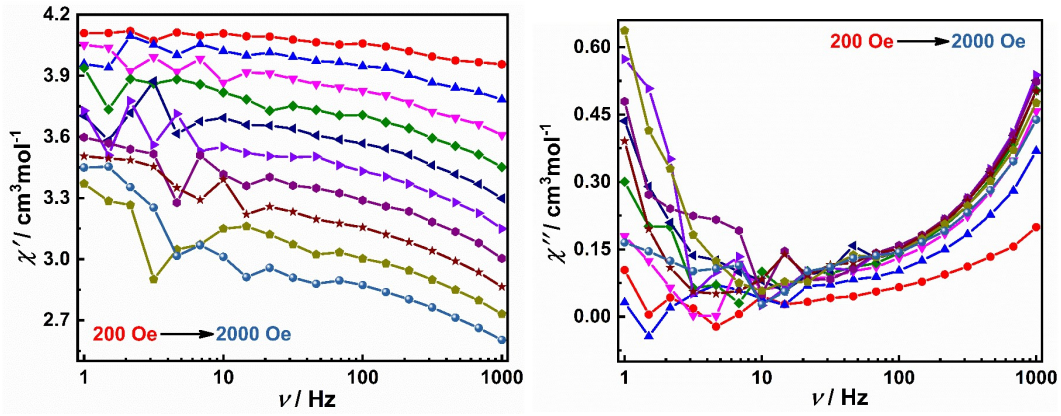
Table S4 Cole-Cole parameters of **1** under 1400 Oe DC field.

T / K	χ_S / cm^{-3} mol^{-1}	χ_T / cm^{-3} mol^{-1}	τ / s	α	R
4	1.48E-01	3.11E+00	5.38E-02	3.58E-01	1.71E-02
4.5	1.45E-01	2.82E+00	2.33E-02	3.50E-01	1.17E-02
5	1.47E-01	2.49E+00	1.03E-02	3.39E-01	8.29E-03
5.5	1.58E-01	2.28E+00	5.30E-03	3.37E-01	1.79E-02
6	1.70E-01	2.09E+00	2.85E-03	3.41E-01	1.13E-02
6.5	1.98E-01	1.94E+00	1.65E-03	3.48E-01	1.34E-02
7	2.50E-01	1.80E+00	1.00E-03	3.47E-01	1.62E-02
7.5	2.98E-01	1.68E+00	6.16E-04	3.55E-01	1.43E-02
8	3.36E-01	1.58E+00	3.83E-04	3.68E-01	9.28E-03
8.5	4.03E-01	1.49E+00	2.55E-04	3.78E-01	1.02E-02
9	4.64E-01	1.40E+00	1.71E-04	3.60E-01	8.66E-03
9.5	4.73E-01	1.33E+00	1.03E-04	3.70E-01	7.58E-03
10	4.53E-01	1.26E+00	5.81E-05	3.69E-01	7.63E-03



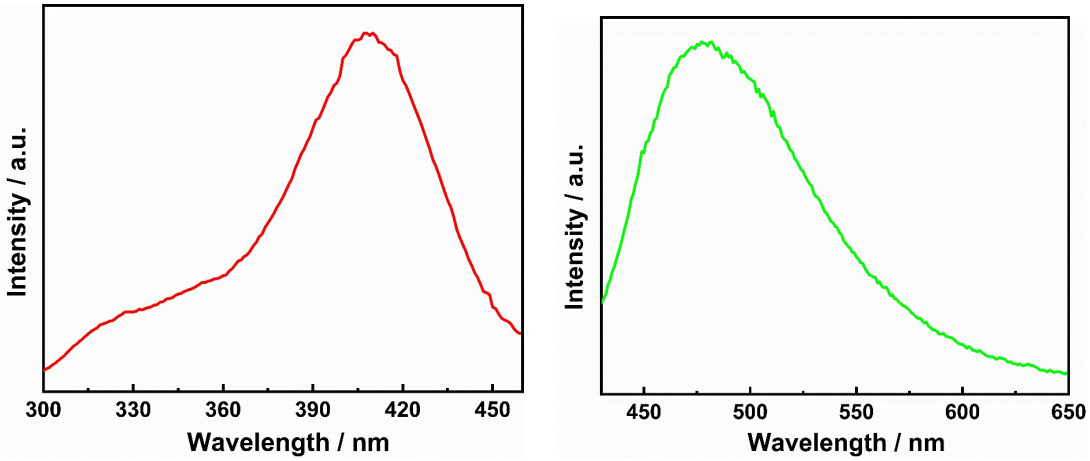
(a) (b)

Fig. S9 Frequency dependence of in-phase (a) and out-of-phase (b) AC susceptibility signals under different DC fields at 2 K for **2**.



(a) (b)

Fig. S10 Frequency dependence of in-phase (a) and out-of-phase (b) AC susceptibility signals under different DC fields at 2 K for **3**.



(a) (b)

Fig. S11 Excitation (a) and emission spectra (b) of the TTP ligand.

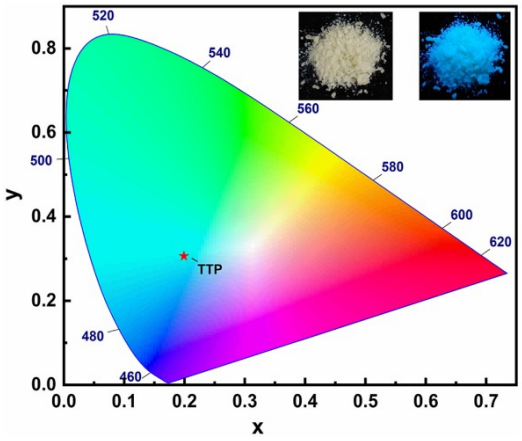
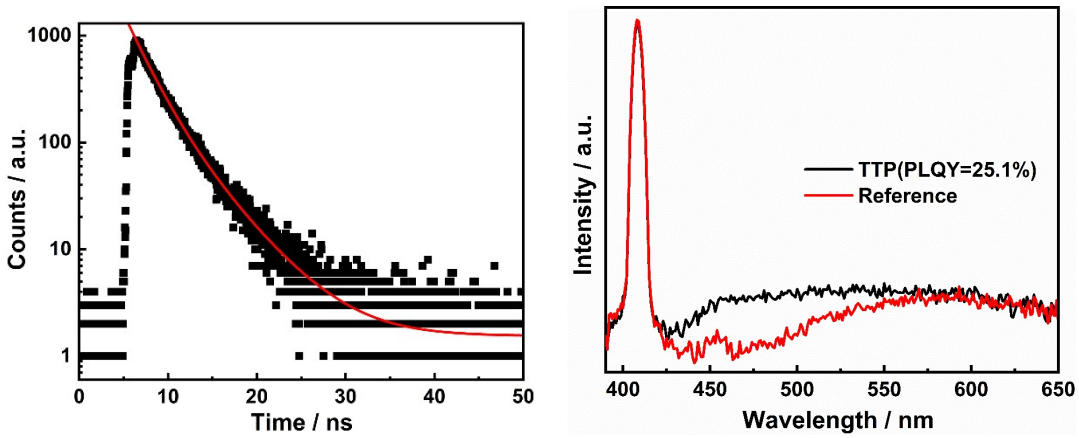
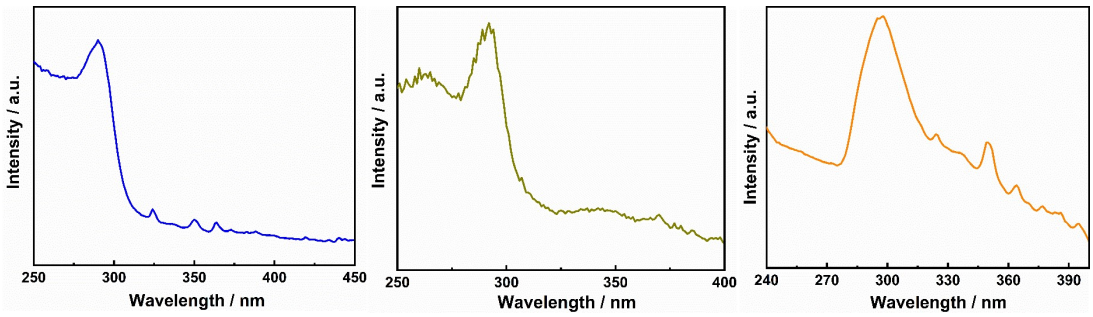


Fig. S12 CIE chromaticity diagrams for the TTP ligand, inset: Images of TTP under day light and UV light.

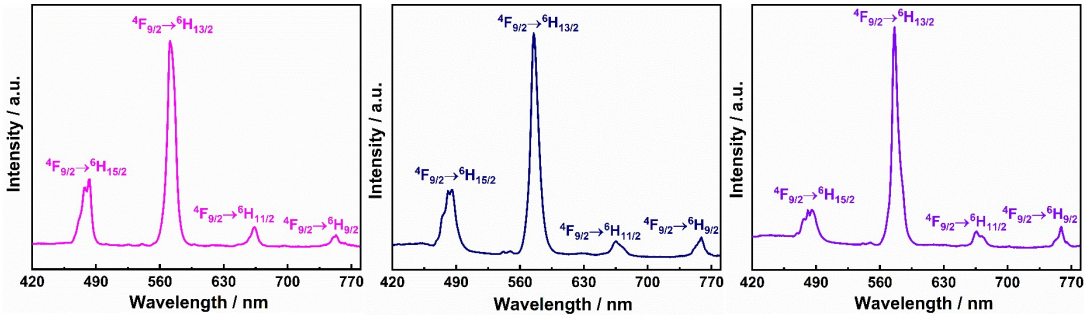


(a) (b)

Fig. S13 (a) Lifetime decay curves for the TTP ligand. (b) Quantum yield of the TTP ligand evaluated with the integrating sphere.

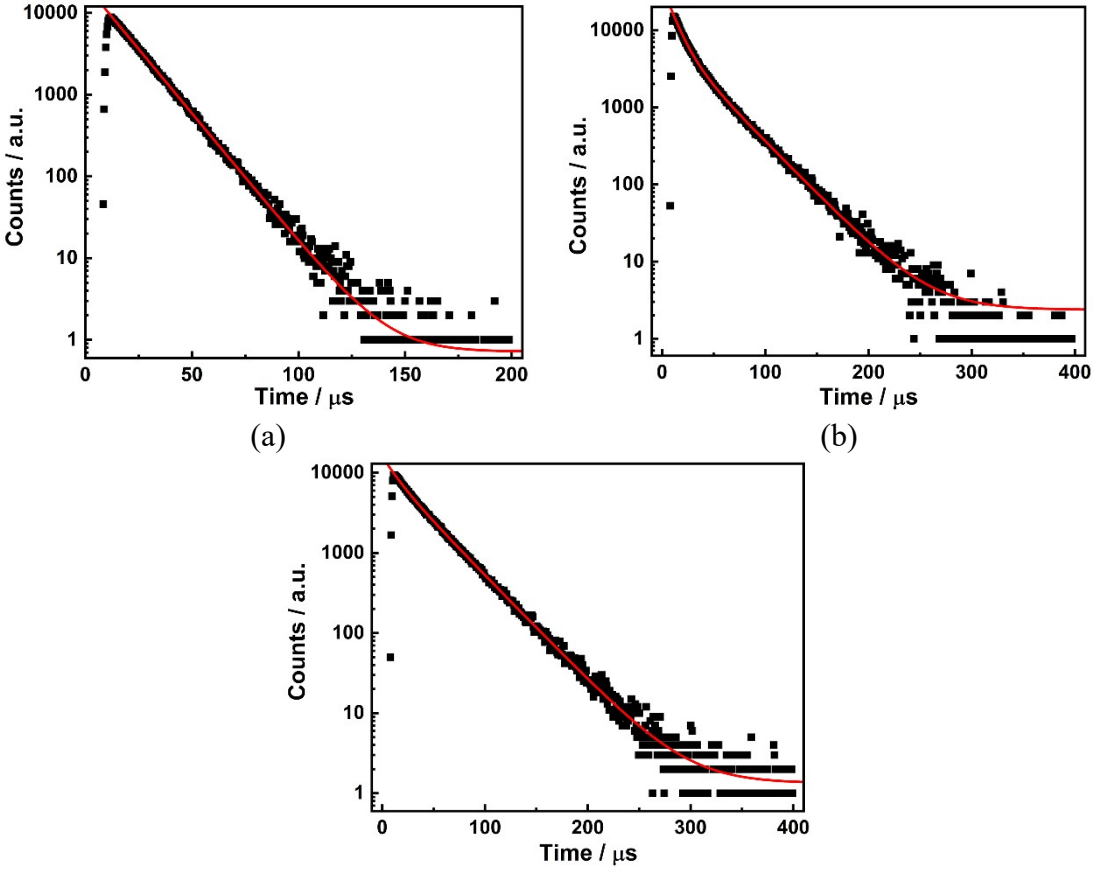


(a) (c) (e)



(b) (d) (f)

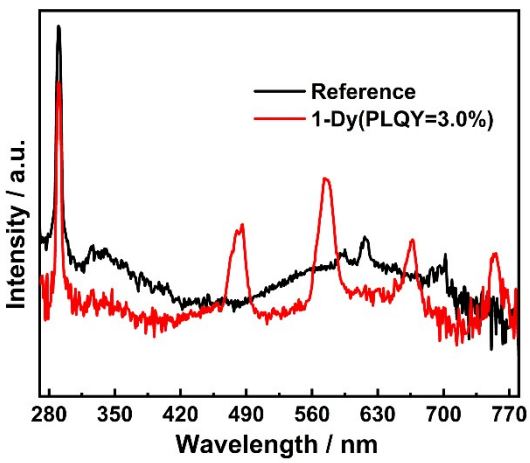
Fig. S14 Excitation and emission spectra of **1** (a, b), **2** (c, d) and **3** (e, f).



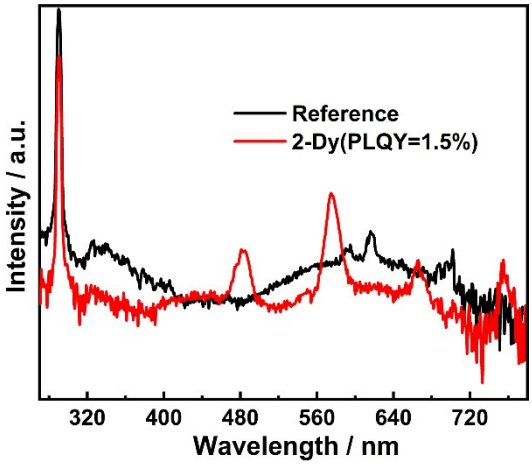
(a) (b)

(c)

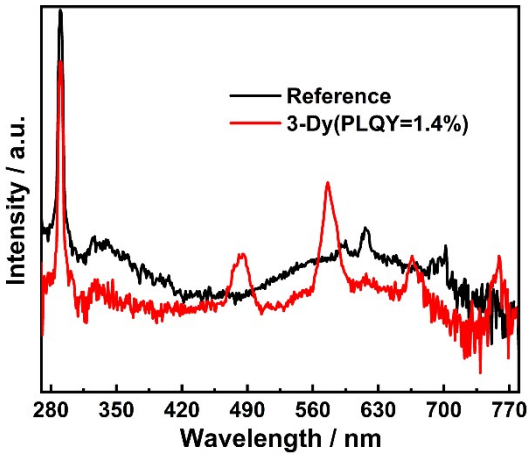
Fig. S15 Lifetime decay curves for **1** (a), **2** (b) and **3** (c). The red line is the best fit to a double exponential function.



(a)

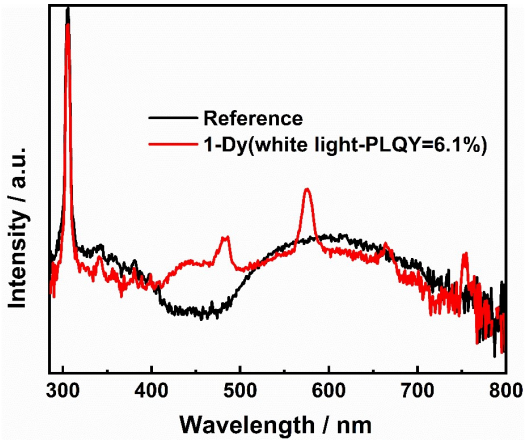


(b)

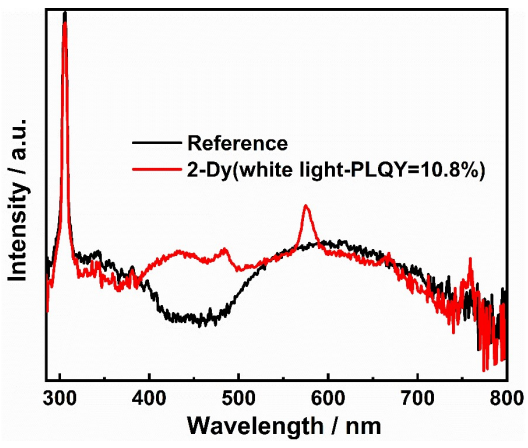


(c)

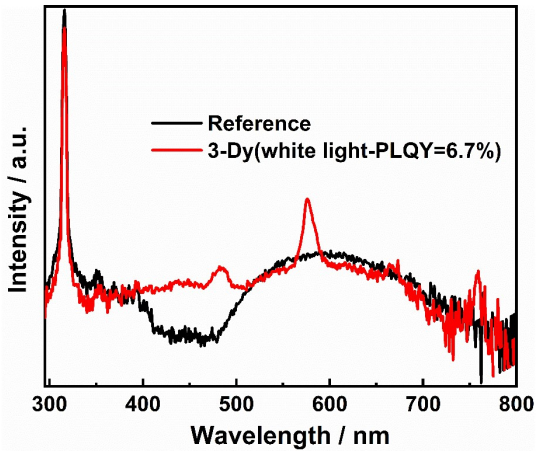
Fig. S16 Yellow light quantum yields of **1** (a), **2** (b) and **3** (c) measured under the excitations of 290, 292, and 297 nm, respectively. Experimental errors of quantum yield: ±10%.



(a)

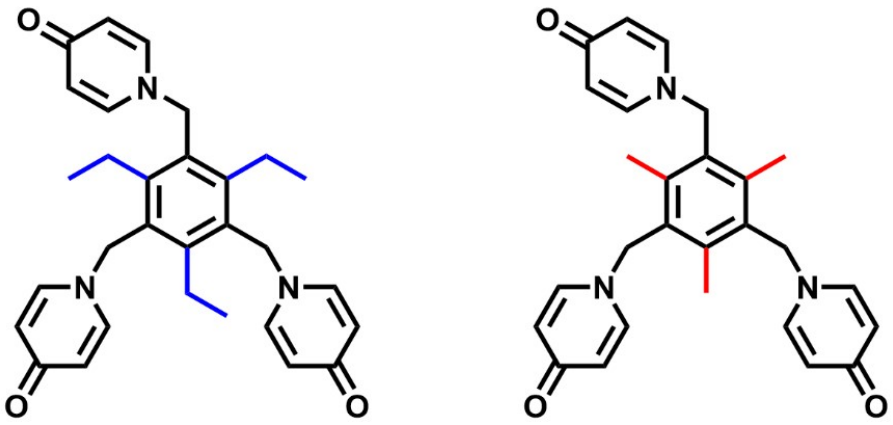


(b)



(c)

Fig. S17 White light quantum yields of **1** (a), **2** (b) and **3** (c) measured under the excitations of 305, 305 and 315 nm, respectively. Experimental errors of quantum yield: ±10%.



(a) (b)

Scheme S1 TETP (a) and TTP (b) ligands.