Supporting Information

Two novel 3D lanthanide supramolecular coordination polymers constructed by paddle wheel SBUs and hydrogen bonding: synthesis, structures and properties

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Table S1 Pertinent Crystal Data and Structure Refinement Results for **1**

Compounds	**1**
CCDC	874175
Formula	$C_{40}H_{28}N_3O_{17}Tb_2$
M_r(g mol^{-1})	1140.49
Space group	*P*-1
***a* (Å)**	13.1321 (2)
***b* (Å)**	13.8370 (7)
***c* (Å)**	16.1264 (2)
α (deg)	75.574 (14)
β (deg)	66.288 (8)
γ (deg)	82.251 (15)
***V* (Å^3)**	2596.35 (14)
Z	2
***D*$_c$ (g cm^{-3})**	1.459
***μ*(mm^{-1})**	2.765
***F*(000)**	1110.0
GOF	1.077
***R*$_1$[a]**	0.0275
***wR*$_2$[a]**	0.0730

$R = \sum (||F_o| - |F_c||)/\sum |F_o|$, $wR = \{ \sum w[(F_o^2 - F_c^2)^2]/ \sum w[(F_o^2)^2]\}^{1/2}$; $[F_o > 4(F_o)]$.

Table S2 Selected bond lengths (Å) and angles (°) for **1**

Tb1—O3^{i}	2.310 (3)	O1—Tb2^{vii}	2.375 (3)
Tb1—O10^{ii}	2.311 (3)	O2—Tb2^{i}	2.295 (2)
Tb1—O4	2.330 (3)	O3—Tb1^{i}	2.310 (3)
Tb1—O9^{iii}	2.390 (3)	O5—Tb2^{v}	2.301 (2)
Tb1—O13	2.416 (3)	O10—Tb1^{ii}	2.311 (3)
Tb1—O16	2.429 (2)	O7—Tb1^{viii}	2.447 (3)
Tb1—O7^{iv}	2.447 (3)	O8—Tb1^{viii}	2.467 (3)
Tb1—O8^{iv}	2.467 (3)	C26—Tb1^{viii}	2.804 (4)
Tb1—C26^{iv}	2.804 (4)	O9—Tb1^{ix}	2.390 (3)
Tb2—O2^{i}	2.295 (2)	Tb2—O6	2.389 (3)
Tb2—O5^{v}	2.301 (2)	Tb2—O11	2.426 (3)
Tb2—O15	2.366 (3)	Tb2—O14	2.462 (3)
Tb2—O1^{vi}	2.375 (3)	Tb2—O12	2.472 (3)
O3^{i}—Tb1—O10^{ii}	76.55 (10)	Tb2—O15—H15B	123.7
O3^{i}—Tb1—O4	121.95 (10)	H15—O15—H15B	107.1
O10^{ii}—Tb1—O4	76.01 (10)	Tb1—O16—H16A	100.2
O3^{i}—Tb1—O9^{iii}	75.31 (10)	Tb1—O16—H16B	124.6
O10^{ii}—Tb1—O9^{iii}	122.43 (9)	C26—O8—Tb1^{viii}	91.6 (2)
O4—Tb1—O9^{iii}	78.09 (10)	C38—O9—Tb1^{ix}	127.2 (2)
O3^{i}—Tb1—O13	78.14 (10)	C38—O10—Tb1^{ii}	155.3 (3)
O10^{ii}—Tb1—O13	78.23 (10)	C39—O11—Tb2	93.3 (2)
O4—Tb1—O13	141.57 (11)	C39—O12—Tb2	91.5 (2)
O9^{iii}—Tb1—O13	140.29 (10)	C40—O13—Tb1	136.7 (3)
O3^{i}—Tb1—O16	83.06 (9)	C40—O14—Tb2	140.1 (3)
O10^{ii}—Tb1—O16	146.03 (9)	Tb2—O15—H15	125.4
O4—Tb1—O16	137.90 (10)	O1^{vi}—Tb2—O6	79.75 (10)

O9^{iii}—Tb1—O16	76.79 (9)	O6—Tb2—O11	134.55 (8)
O13—Tb1—O16	71.11 (9)	O2^{i}—Tb2—O14	75.85 (10)
O3^{i}—Tb1—O7^{iv}	150.48 (9)	O5^{v}—Tb2—O14	75.34 (10)
O10^{ii}—Tb1—O7^{iv}	132.88 (9)	O15—Tb2—O14	72.53 (9)
O4—Tb1—O7^{iv}	72.43 (10)	O1^{vi}—Tb2—O14	140.21 (10)
O9^{iii}—Tb1—O7^{iv}	83.93 (9)	O6—Tb2—O14	139.63 (10)
O13—Tb1—O7^{iv}	106.89 (10)	O11—Tb2—O14	75.36 (10)
O16—Tb1—O7^{iv}	71.78 (9)	O2^{i}—Tb2—O12	149.42 (9)
O3^{i}—Tb1—O8^{iv}	150.15 (10)	O5^{v}—Tb2—O12	131.39 (9)
O10^{ii}—Tb1—O8^{iv}	85.64 (10)	O15—Tb2—O12	73.34 (9)
O4—Tb1—O8^{iv}	75.18 (10)	O1^{vi}—Tb2—O12	69.59 (9)
O9^{iii}—Tb1—O8^{iv}	134.44 (9)	O6—Tb2—O12	82.22 (9)
O13—Tb1—O8^{iv}	74.86 (10)	O11—Tb2—O12	53.30 (9)
O16—Tb1—O8^{iv}	99.82 (9)	O14—Tb2—O12	112.84 (10)
O7^{iv}—Tb1—O8^{iv}	53.09 (9)	O2^{i}—Tb2—C39	166.79 (10)
O3^{i}—Tb1—C26^{iv}	168.73 (10)	O5^{v}—Tb2—C39	109.08 (11)
O10^{ii}—Tb1—C26^{iv}	108.78 (11)	O15—Tb2—C39	85.53 (11)
O4—Tb1—C26^{iv}	69.30 (10)	O1^{vi}—Tb2—C39	69.48 (10)
O9^{iii}—Tb1—C26^{iv}	108.48 (11)	O6—Tb2—C39	108.03 (10)
O13—Tb1—C26^{iv}	93.04 (11)	O11—Tb2—C39	26.84 (10)
O16—Tb1—C26^{iv}	87.48 (10)	O14—Tb2—C39	95.51 (11)
O7^{iv}—Tb1—C26^{iv}	26.49 (10)	O12—Tb2—C39	26.54 (10)
O8^{iv}—Tb1—C26^{iv}	26.83 (10)	C12—O1—Tb2^{vii}	134.2 (2)
O2^{i}—Tb2—O5^{v}	78.75 (10)	C12—O2—Tb2^{i}	152.0 (3)
O2^{i}—Tb2—O15	82.35 (10)	C13—O3—Tb1^{i}	146.0 (2)
O5^{v}—Tb2—O15	145.81 (9)	C13—O4—Tb1	140.4 (2)
O2^{i}—Tb2—O1^{vi}	123.49 (10)	C25—O5—Tb2^{v}	162.2 (2)
O5^{v}—Tb2—O1^{vi}	75.49 (10)	C25—O6—Tb2	122.1 (2)

O15—Tb2—O1^{vi}	138.35 (9)	C26—O7—Tb1^{viii}	92.9 (2)
O2^{i}—Tb2—O6	74.34 (10)	O5^{v}—Tb2—O6	123.69 (9)
O15—Tb2—O6	77.05 (10)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) −*x*+2, −*y*+1, −*z*; (iii) *x*, *y*−1, *z*; (iv) *x*+1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*; (vi) *x*−1, *y*+1, *z*; (vii) *x*+1, *y*−1, *z*; (viii) *x*−1, *y*, *z*; (ix) *x*, *y*+1, *z*.

Table S3 Bond lengths (Å) and angles (º) of hydrogen bonds for **1**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1-H1*B*···O16^{iii}	0.86	2.09	2.788 (4)	138
O15-H15···O13	0.85	2.00	2.750 (4)	147
O15-H15···O16	0.85	2.60	3.283(4)	138
O15-H15*B*···N3^{i}	0.85	1.92	2.750 (4)	166
O16-H16*B*···N2^{ii}	0.85	2.03	2.874 (5)	170

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*+1, *y*, *z*.

Table S4 Quantum yields and lifetimes of **1** and **2** at 298, 77 and 10 K

Compound	**Temperature (K)**	**Lifetime(ms)**		**Quantum Yields Φ_f[c]**	**λ_{ex}(nm)**
		τ_1	**τ_2**		

	298	0.6935(85.04%)	0.1876(14.96%)	17.40%	310
1	77	0.9778(93.43%)	0.3116(6.57%)	39.05%	310
	10	1.0000(100%)	0	44.66%	310
	298	0.7653(67.18%)	0.3264(32.82%)	5.49%	338
2	77	1.086(81.36%)	0.3480(18.64%)	22.84%	338
	10	1.185(96.03%)	0.372(3.97%)	26.75%	338

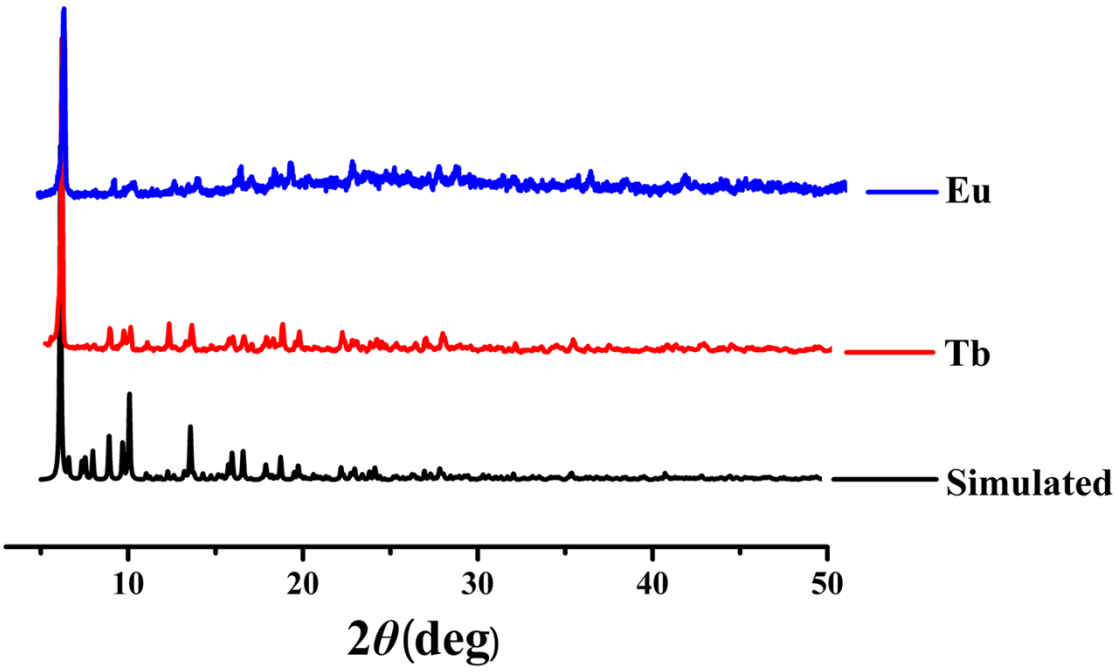

Fig. S1 X-ray powder diffraction (XRPD) patterns of **1** (Tb) and **2** (Eu)

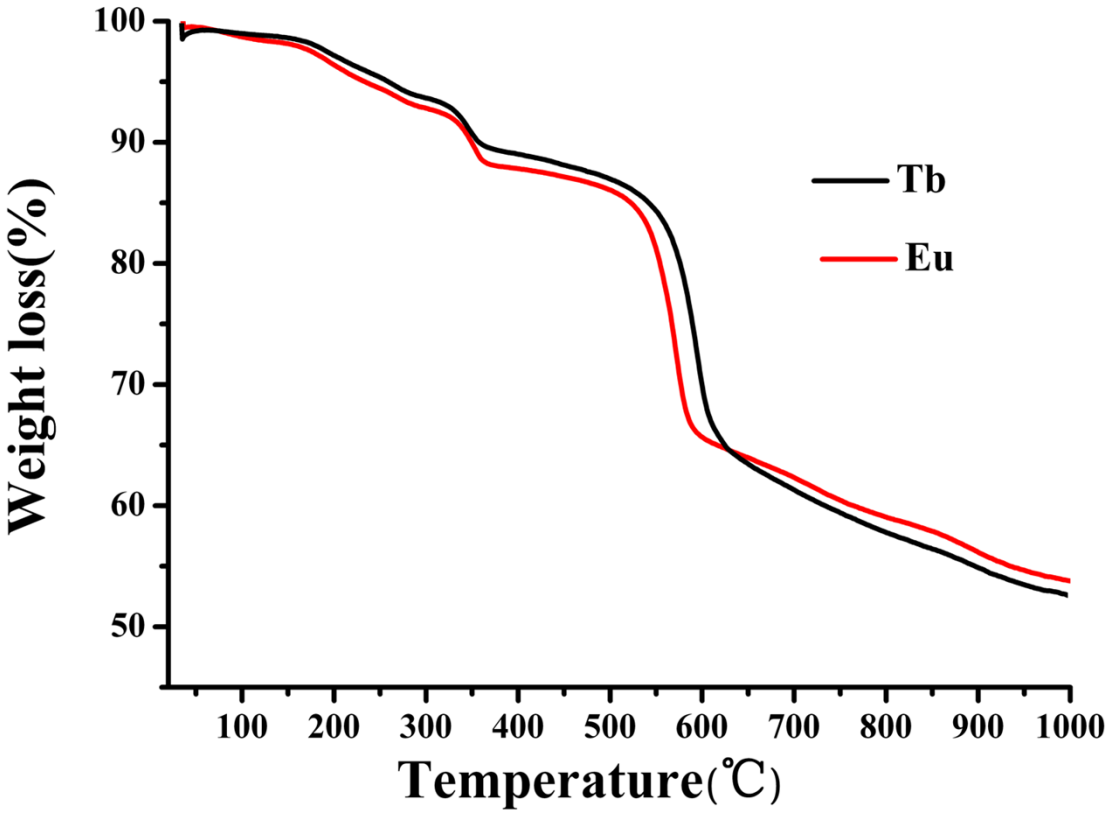

Fig. S2 View of the TGA curves of **1** (Tb) and **2** (Eu)

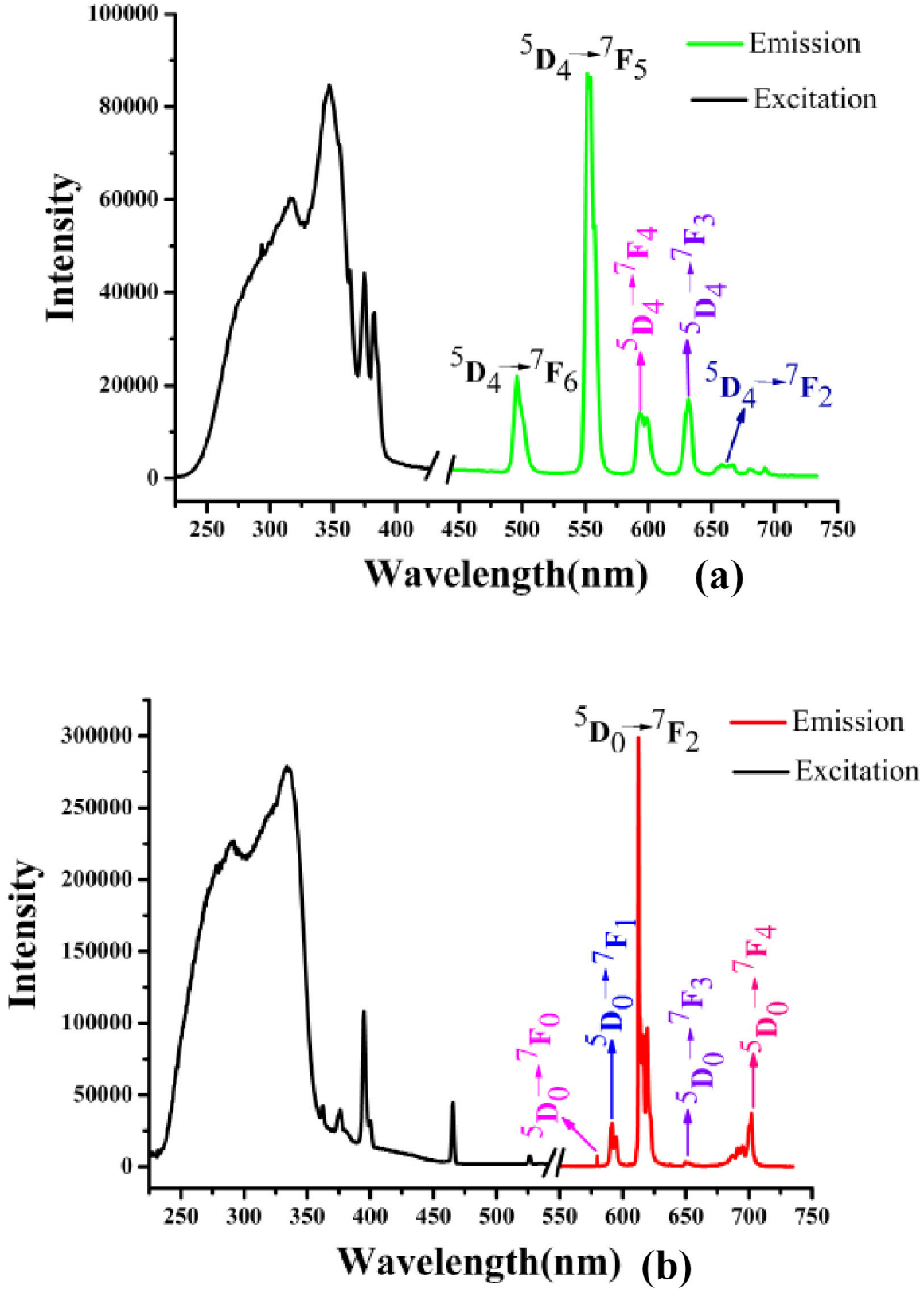

Fig S3 Solid-state excitation and emission spectra for **1** (a) and **2** (b) at room temperature

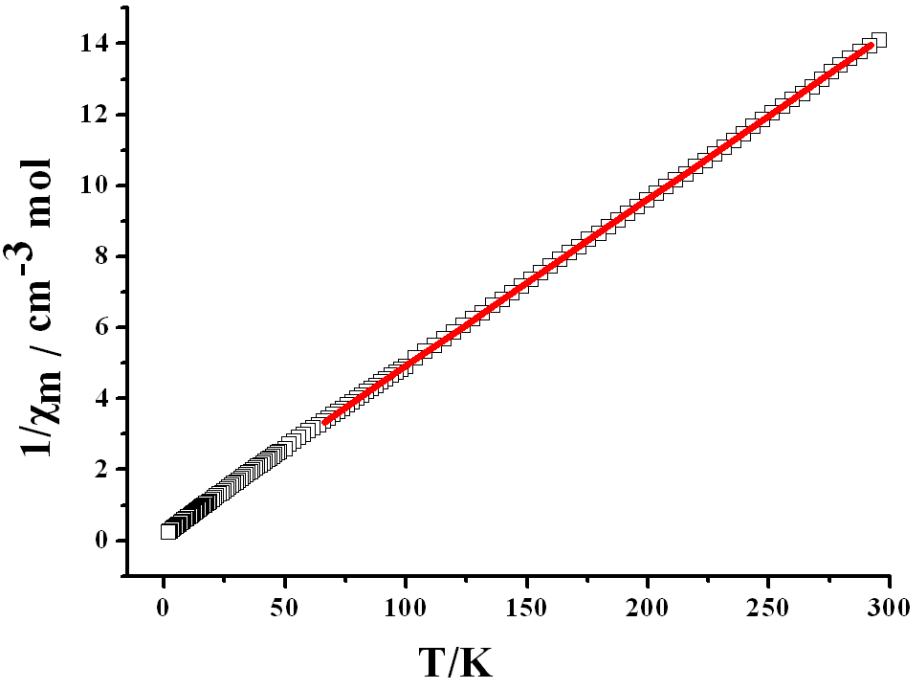

Fig S4 The red line shows the Curie–Weiss fitting for **1.**