Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A family of 3D lanthanide organic frameworks with tunable luminescence and slow magnetic relaxation

Qipeng Li,[a,b] and Shaowu Du*[a]

[a] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, PR China*

[b] *Graduate University of Chinese Academy of Sciences, Beijing 100039, PR China*

Table S1 Selected bond lengths (Å) and angles (º) for Compound **1**

Compound **1**			
Sm1—O13^{i}	2.35 (2)	O8—Sm1^{iv}	2.572 (12)
Sm1—O3^{i}	2.370 (4)	O13—Sm1^{v}	2.35 (2)
Sm1—O1^{ii}	2.377 (4)	O1—Sm1^{ii}	2.377 (4)
Sm1—O4^{iii}	2.389 (4)	O7—Sm1^{iv}	2.479 (14)
Sm1—O2	2.423 (4)	O3—Sm1^{v}	2.370 (4)
Sm1—O9	2.450 (4)	O4—Sm1^{vi}	2.389 (4)
Sm1—O7^{iv}	2.479 (14)	Sm1—O10	2.49 (2)
Sm1—O6	2.483 (14)	Sm1—O5	2.55 (2)
Sm1—O1	2.788 (4)	Sm1—O8^{iv}	2.572 (12)
O13^{i}—Sm1—O3^{i}	69.7 (4)	O6^{iv}—O7—Sm1^{iv}	84 (3)
O13^{i}—Sm1—O1^{ii}	77.6 (5)	C26—O7—Sm1^{iv}	94.1 (8)
O3^{i}—Sm1—O1^{ii}	75.80 (15)	C14^{iv}—O7—Sm1^{iv}	83.1 (6)
O13^{i}—Sm1—O4^{iii}	131.1 (4)	C26—O8—Sm1^{iv}	90.0 (7)
O3^{i}—Sm1—O4^{iii}	133.41 (13)	O5—C14—Sm1	62.9 (11)
O1^{ii}—Sm1—O4^{iii}	71.33 (15)	O6—C14—Sm1	59.9 (8)
O13^{i}—Sm1—O2	136.4 (4)	C15—C14—Sm1	179.2 (7)
O3^{i}—Sm1—O2	78.88 (19)	O7^{iv}—C14—Sm1	59.3 (5)
O1^{ii}—Sm1—O2	123.32 (14)	O8—C26—Sm1^{iv}	63.9 (7)
O4^{iii}—Sm1—O2	92.5 (2)	O7—C26—Sm1^{iv}	59.7 (7)
O13^{i}—Sm1—O9	69.4 (5)	C17—C26—Sm1^{iv}	174.3 (7)
O3^{i}—Sm1—O9	79.88 (13)	O6^{iv}—C26—Sm1^{iv}	59.3 (5)
O1^{ii}—Sm1—O9	144.21 (15)	O4^{iii}—Sm1—O6	77.5 (4)
O4^{iii}—Sm1—O9	142.61 (14)	O2—Sm1—O6	128.6 (3)
O2—Sm1—O9	76.06 (17)	O9—Sm1—O6	82.3 (4)

O13^{i}—Sm1—O7^{iv}	60.9 (4)	O7^{iv}—Sm1—O6	12.0 (2)
O3^{i}—Sm1—O7^{iv}	130.5 (2)	O13^{i}—Sm1—O10	122.4 (7)
O1^{ii}—Sm1—O7^{iv}	94.8 (4)	O3^{i}—Sm1—O10	138.6 (4)
O4^{iii}—Sm1—O7^{iv}	84.8 (3)	O1^{ii}—Sm1—O10	142.4 (5)
O2—Sm1—O7^{iv}	138.7 (3)	O4^{iii}—Sm1—O10	72.0 (6)
O9—Sm1—O7^{iv}	81.5 (4)	O2—Sm1—O10	66.4 (3)
O13^{i}—Sm1—O6	72.4 (4)	O9—Sm1—O10	70.7 (6)
O3^{i}—Sm1—O6	141.8 (3)	O7^{iv}—Sm1—O10	73.7 (4)
O1^{ii}—Sm1—O6	101.1 (3)	O6—Sm1—O10	62.5 (4)
O5—Sm1—O8^{iv}	110.8 (4)	O13^{i}—Sm1—O5	116.4 (6)
O13^{i}—Sm1—O1	133.1 (5)	O3^{i}—Sm1—O5	148.7 (4)
O3^{i}—Sm1—O1	67.22 (14)	O1^{ii}—Sm1—O5	135.0 (5)
O1^{ii}—Sm1—O1	74.57 (13)	O4^{iii}—Sm1—O5	68.0 (5)
O4^{iii}—Sm1—O1	72.78 (14)	O2—Sm1—O5	77.4 (3)
O2—Sm1—O1	48.87 (13)	O9—Sm1—O5	74.7 (5)
O9—Sm1—O1	118.98 (14)	O7^{iv}—Sm1—O5	63.3 (3)
O7^{iv}—Sm1—O1	157.2 (3)	O6—Sm1—O5	51.9 (3)
O6—Sm1—O1	149.8 (3)	O10—Sm1—O5	11.2 (4)
O10—Sm1—O1	102.3 (5)	O13^{i}—Sm1—O8^{iv}	10.1 (5)
O5—Sm1—O1	110.0 (4)	O3^{i}—Sm1—O8^{iv}	79.0 (2)
O8^{iv}—Sm1—O1	139.1 (3)	O1^{ii}—Sm1—O8^{iv}	75.4 (3)
C1—O1—Sm1^{ii}	165.4 (4)	O4^{iii}—Sm1—O8^{iv}	121.8 (3)
C1—O1—Sm1	85.9 (3)	O2—Sm1—O8^{iv}	145.6 (3)
Sm1^{ii}—O1—Sm1	105.43 (13)	O9—Sm1—O8^{iv}	74.4 (4)
C1—O2—Sm1	103.3 (4)	O7^{iv}—Sm1—O8^{iv}	51.9 (2)
C13—O3—Sm1^{v}	141.3 (4)	O6—Sm1—O8^{iv}	63.8 (3)
C13—O4—Sm1^{vi}	138.7 (4)	O10—Sm1—O8^{iv}	118.4 (5)
O1—C1—Sm1	69.3 (3)	C14—O5—Sm1	91.1 (12)

O2—C1—Sm1	52.5 (3)	O7^{iv}—O6—Sm1	84 (3)
C2—C1—Sm1	165.9 (5)	C14—O6—Sm1	94.2 (8)
C26^{iv}—O6—Sm1	82.8 (6)		

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*, *y*+1/2, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*, −*y*+1/2, *z*+1/2; (vi) −*x*, *y*−1/2, −*z*+3/2; (vii) −*x*+1, −*y*+1, −*z*+2.

Table S2 Selected bond lengths (Å) and angles (º) for Compound **5**

Compound **5**			
Dy1—O1^{i}	2.304 (3)	O8—Dy1^{iv}	2.562 (19)
Dy1—O3^{ii}	2.328 (3)	C26—Dy1^{iv}	2.833 (7)
Dy1—O4^{iii}	2.339 (3)	O13—Dy1^{v}	2.38 (2)
Dy1—O2	2.366 (3)	Dy1—O5	2.475 (16)
Dy1—O13^{ii}	2.38 (2)	Dy1—O8^{iv}	2.56 (2)
Dy1—O9	2.384 (3)	O1—Dy1^{i}	2.304 (3)
Dy1—O7^{iv}	2.411 (12)	O3—Dy1^{v}	2.328 (3)
Dy1—O6	2.442 (13)	O4—Dy1^{vi}	2.339 (3)
Dy1—O10	2.450 (16)	O7—Dy1^{iv}	2.411 (12)
O1^{i}—Dy1—O3^{ii}	77.59 (12)		
O1^{i}—Dy1—O4^{iii}	72.12 (12)	O6^{iv}—O7—Dy1^{iv}	88 (3)
O3^{ii}—Dy1—O4^{iii}	131.39 (10)	C26—O7—Dy1^{iv}	95.7 (6)
O1^{i}—Dy1—O2	123.39 (12)	C14^{iv}—O7—Dy1^{iv}	84.7 (5)
O3^{ii}—Dy1—O2	78.87 (13)	C26—O8—Dy1^{iv}	89.1 (10)
O4^{iii}—Dy1—O2	87.06 (14)	O5—C14—Dy1	61.8 (8)
O1^{i}—Dy1—O13^{ii}	77.8 (7)	O6—C14—Dy1	60.3 (7)
O3^{ii}—Dy1—O13^{ii}	72.1 (4)	C15—C14—Dy1	179.6 (6)
O4^{iii}—Dy1—O13^{ii}	133.8 (6)	O7^{iv}—C14—Dy1	58.8 (4)
O2—Dy1—O13^{ii}	139.1 (5)	O9—Dy1—C14	79.93 (18)

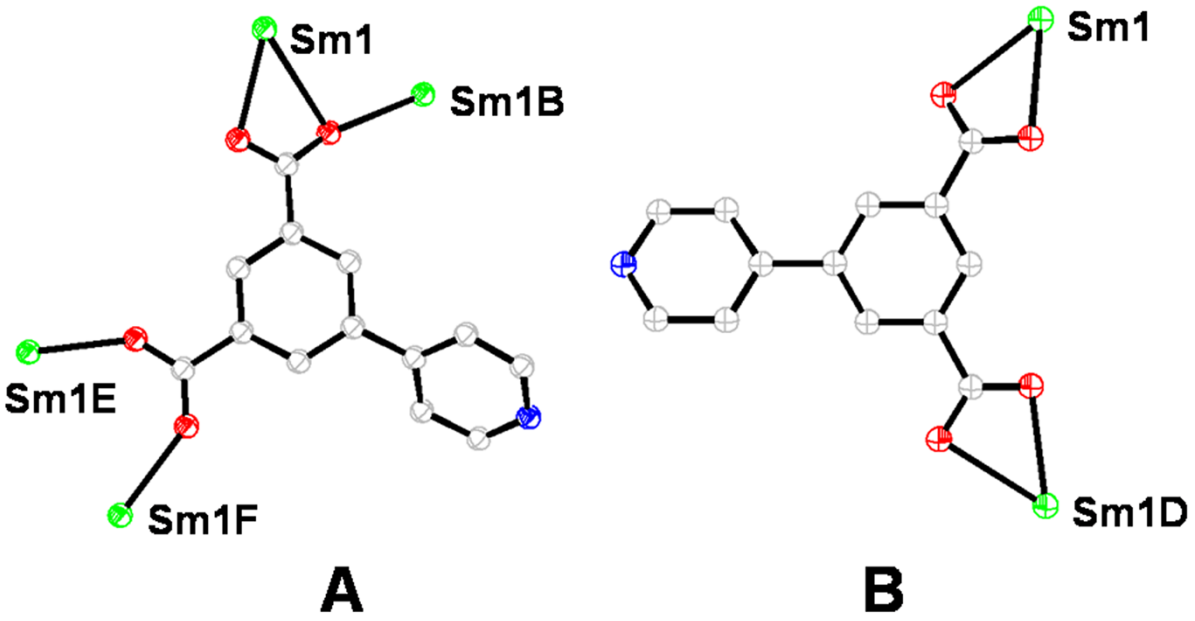
O1^{i}—Dy1—O9	145.48 (13)	O7^{iv}—Dy1—C14	36.5 (2)
O3^{ii}—Dy1—O9	79.88 (11)	O6—Dy1—C14	26.53 (19)
O4^{iii}—Dy1—O9	141.33 (12)	O10—Dy1—C14	37.5 (3)
O2—Dy1—O9	76.62 (14)	O5—Dy1—C14	26.54 (18)
O13^{ii}—Dy1—O9	70.5 (7)	O8^{iv}—Dy1—C14	86.8 (3)
O1^{i}—Dy1—O7^{iv}	91.7 (3)	C1—O1—Dy1^{i}	172.1 (3)
O3^{ii}—Dy1—O7^{iv}	131.01 (17)	C1—O2—Dy1	108.1 (3)
O4^{iii}—Dy1—O7^{iv}	87.4 (2)	C13—O3—Dy1^{v}	140.7 (3)
O2—Dy1—O7^{iv}	140.5 (3)	C13—O4—Dy1^{vi}	139.4 (3)
O13^{ii}—Dy1—O7^{iv}	58.9 (4)	O1—C1—Dy1	74.6 (2)
O9—Dy1—O7^{iv}	83.7 (3)	O2—C1—Dy1	48.6 (2)
O1^{i}—Dy1—O6	94.8 (3)	C2—C1—Dy1	162.9 (3)
O3^{ii}—Dy1—O6	142.8 (2)	C14—O5—Dy1	91.7 (9)
O4^{iii}—Dy1—O6	77.7 (3)	O7^{iv}—O6—Dy1	81 (3)
O2—Dy1—O6	132.0 (2)	C14—O6—Dy1	93.2 (7)
O13^{ii}—Dy1—O6	70.7 (4)	C26^{iv}—O6—Dy1	83.0 (5)
O9—Dy1—O6	87.6 (3)	O10—Dy1—O5	11.3 (3)
O7^{iv}—Dy1—O6	11.7 (2)	O1^{i}—Dy1—O8^{iv}	75.6 (5)
O1^{i}—Dy1—O10	141.1 (3)	O3^{ii}—Dy1—O8^{iv}	78.7 (2)
O3^{ii}—Dy1—O10	139.1 (3)	O4^{iii}—Dy1—O8^{iv}	126.9 (4)
O4^{iii}—Dy1—O10	71.7 (4)	O2—Dy1—O8^{iv}	146.0 (4)
O2—Dy1—O10	68.1 (3)	O13^{ii}—Dy1—O8^{iv}	7.4 (7)
O13^{ii}—Dy1—O10	119.5 (7)	O9—Dy1—O8^{iv}	74.6 (5)
O9—Dy1—O10	69.7 (4)	O7^{iv}—Dy1—O8^{iv}	52.5 (3)
O7^{iv}—Dy1—O10	73.1 (3)	O6—Dy1—O8^{iv}	64.2 (3)
O6—Dy1—O10	64.0 (3)	O10—Dy1—O8^{iv}	116.9 (5)
O1^{i}—Dy1—O5	133.1 (3)	O5—Dy1—O8^{iv}	109.5 (4)
O3^{ii}—Dy1—O5	149.0 (3)	O1^{i}—Dy1—C14	115.29 (18)

O4^{iii}—Dy1—O5	68.4 (4)	O3^{ii}—Dy1—C14	157.66 (17)
O2—Dy1—O5	79.0 (2)	O4^{iii}—Dy1—C14	70.95 (18)
O13^{ii}—Dy1—O5	113.3 (6)	O2—Dy1—C14	105.54 (17)
O9—Dy1—O5	74.1 (4)	O13^{ii}—Dy1—C14	92.1 (4)
O7^{iv}—Dy1—O5	62.7 (3)	O6—Dy1—O5	53.1 (3)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*−1/2; (iii) −*x*, *y*+1/2, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*, −*y*+1/2, *z*+1/2; (vi) −*x*, *y*−1/2, −*z*+3/2; (vii) −*x*+1, −*y*+1, −*z*+2.

Table S3 The Quantum yields and lifetimes of compound **2** and **4**

Compound	Temperature (K)	Lifetime(ms) τ_1	Quantum Yields Φ_f[c]	λ_{ex}(nm)
	298	0.3911	17.82%	280
2	77		38.65%	280
	10		48.01%	280
	298	0.8372	43.94%	310
4	77		49.97%	310
	10		56.22%	310



Scheme S1 The coordination modes of PIP^{2-} ligand in compound **1**

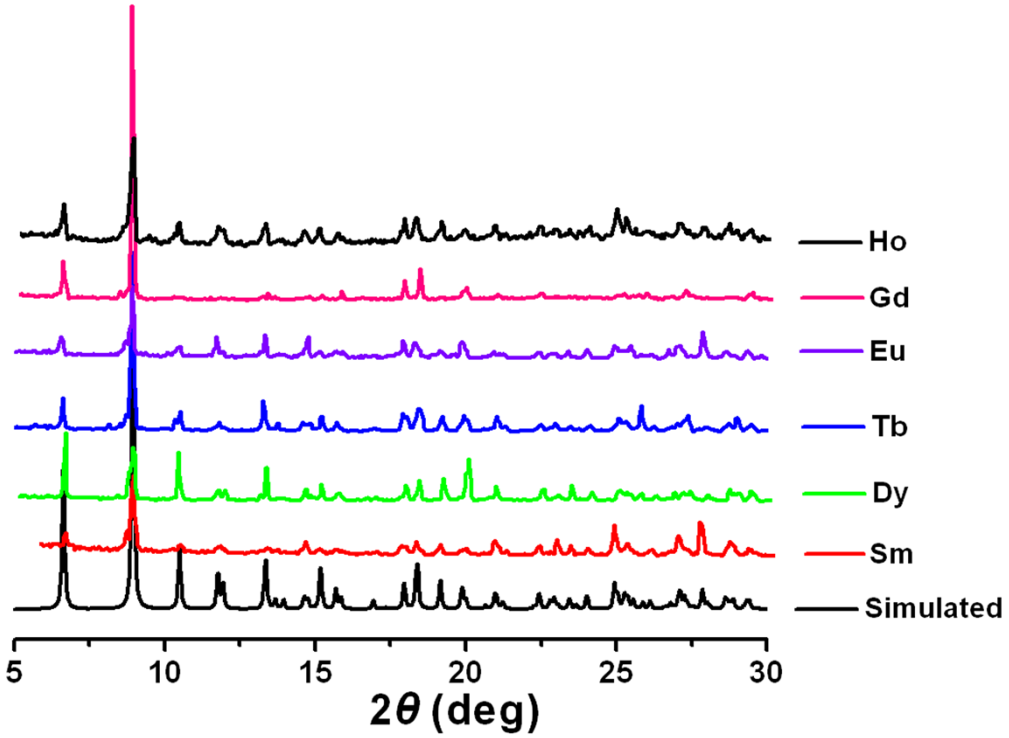


Fig S1 X-ray powder diffraction (XRPD) patterns of compound **1** (Sm), **2** (Eu), **3** (Gd), **4** (Tb), **5** (Dy) and **6** (Ho)

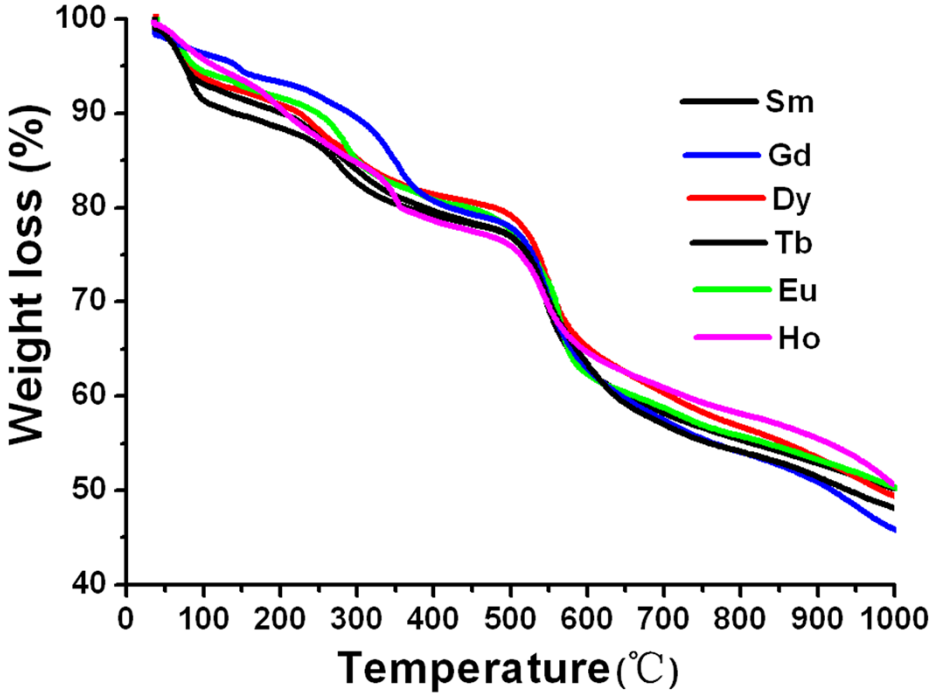


Fig S2 TGA curves of compound **1** (Sm), **2** (Eu), **3** (Gd), **4** (Tb), **5** (Dy) and **6** (Ho)

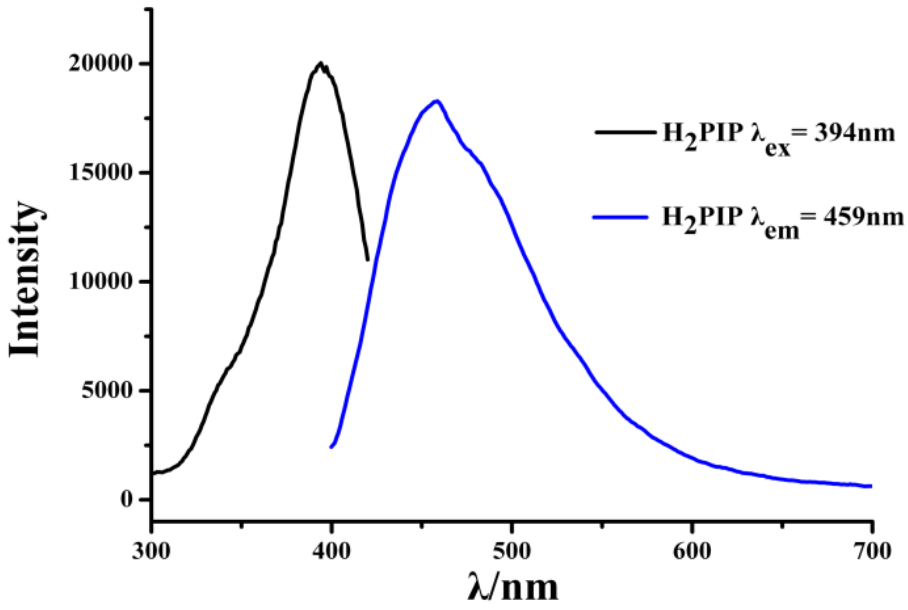


Fig S3 Solid-state excitation and emission spectra for H_2PIP ligand at room temperature

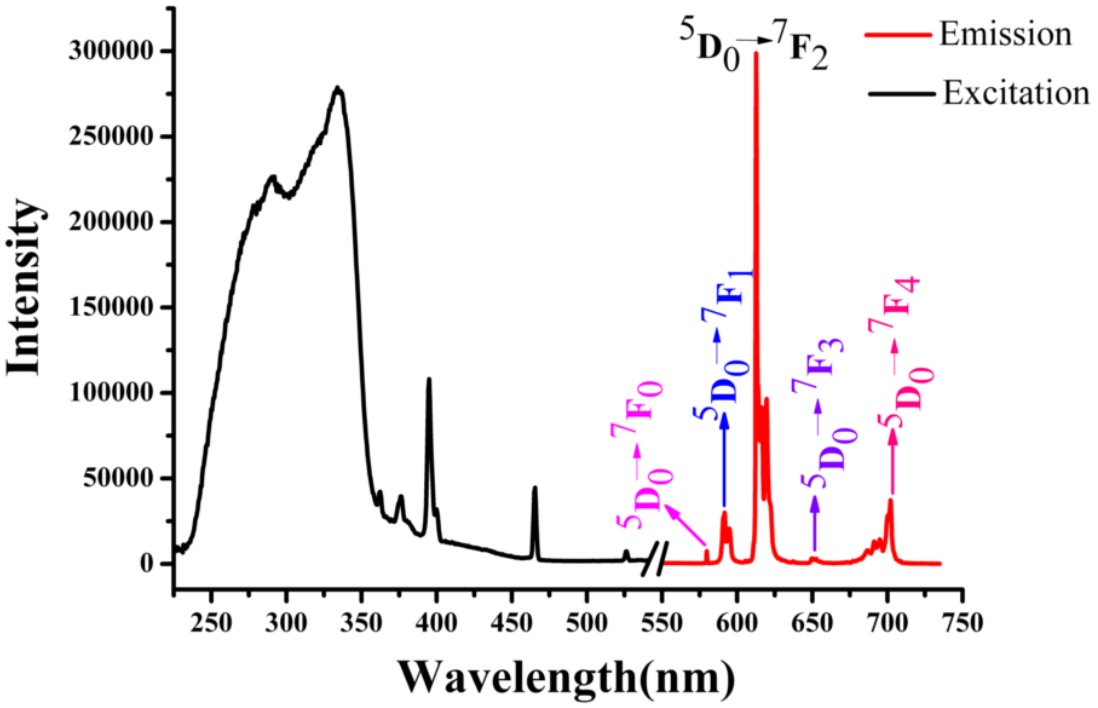


Fig S4 Solid-state excitation and emission spectra for **2** at room temperature

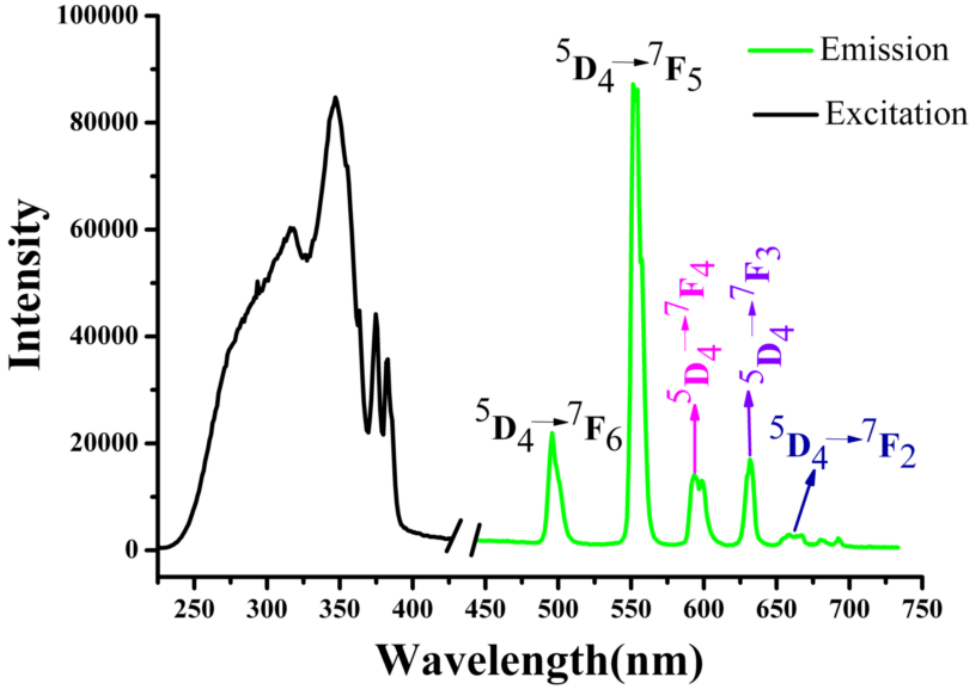


Fig S5 Solid-state excitation and emission spectra for **4** at room temperature

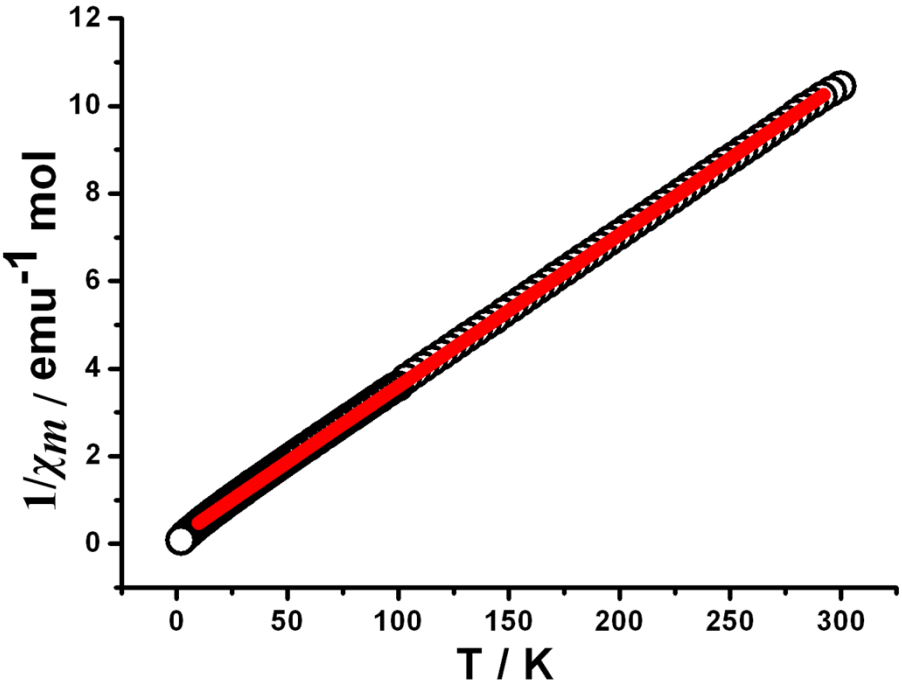


Fig S6 The red line shows the Curie–Weiss fitting for **5-Dy**.

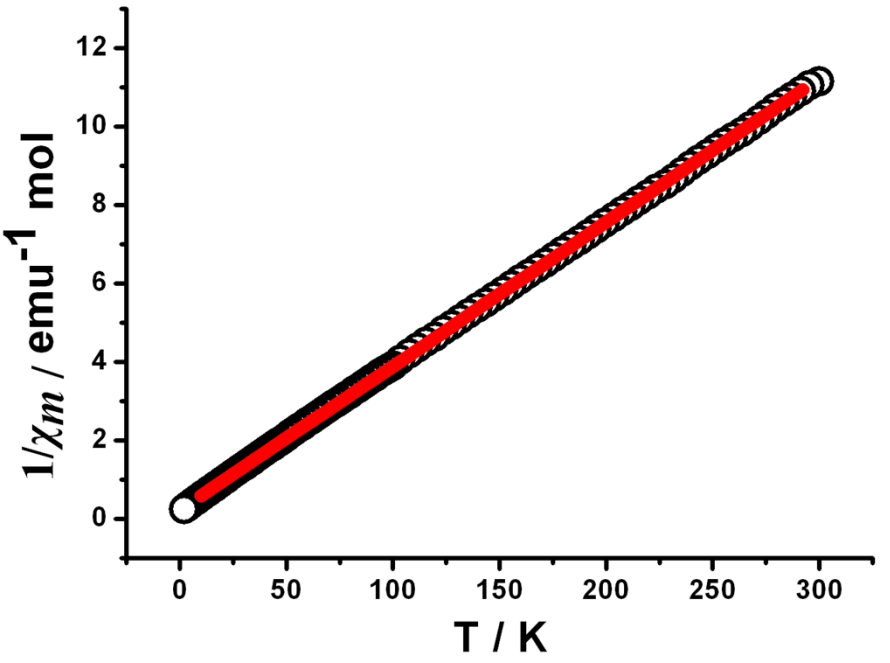


Fig S7 The red line shows the Curie–Weiss fitting for **6-Ho.**

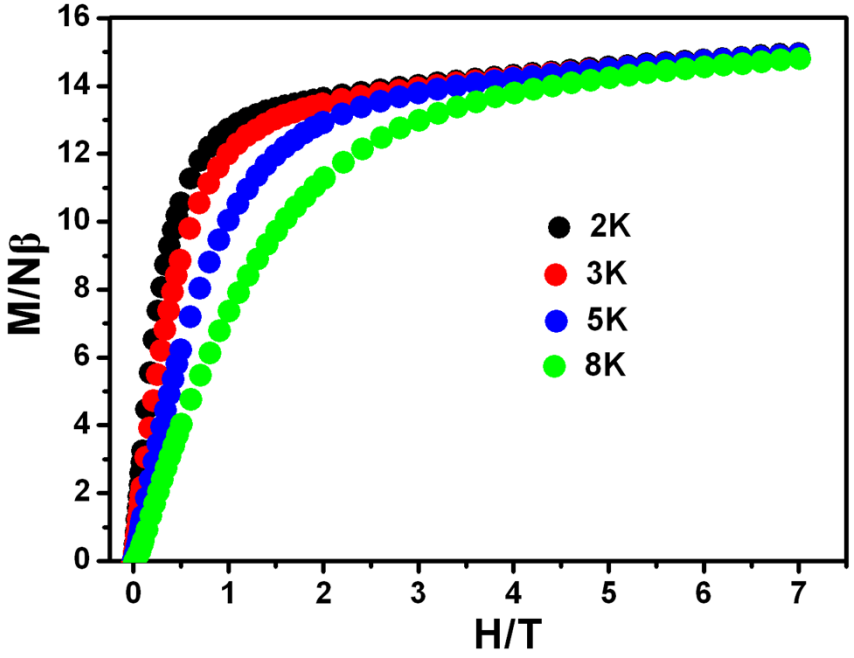


Fig S8 The plot of M-H for **5-Dy.**