Electronic Supplementary Material (ESI) for RSC Advances.

Crystal structures and luminescent properties of new lanthanide(III) complexes derived from 2-phenyl-4-pyrimidinecarboxylate

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Table S1 Selected Bond Lengths (Å) and Bond Angles (deg) for compounds **1-2**.

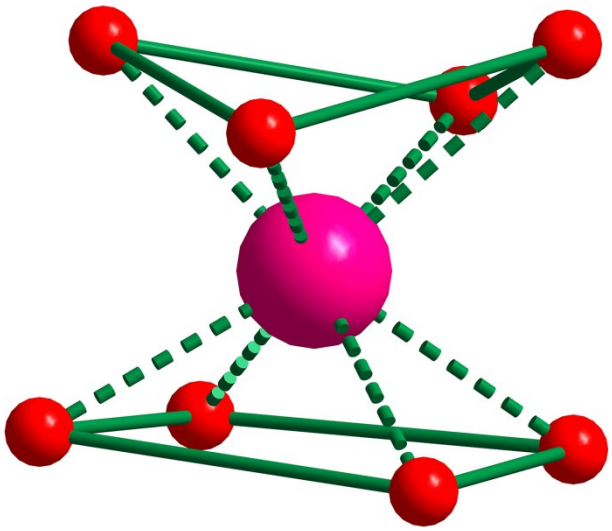
1							
Eu1-O5	2.325(4)	Eu1-O2b	2.343(4)	Eu1-O6b	2.347(4)	Eu1-O1	2.383(4)
Eu1-O7	2.394(4)	Eu1-O8	2.427(5)	Eu1-O3	2.482(4)	Eu1-O4	2.505(4)
O5-Eu1-O2a	84.2(2)	O5-Eu1-O6b	149.3(2)	O2a-Eu1-O6b	77.8(1)		
O5-Eu1-O1	110.3(2)	O2a-Eu1-O1	149.0(2)	O6b-Eu1-O1	76.3(2)		
O5-Eu1-O7	70.7(1)	O2a-Eu1-O7	81.7(2)	O6b-Eu1-O7	82.0(2)		
O1-Eu1-O7	78.1(2)	O5-Eu1-O8	76.9(2)	O2a-Eu1-O8	145.5(4)		
O6b-Eu1-O8	130.1(2)	O1-Eu1-O8	65.5(2)	O7-Eu1-O8	117.7(2)		
O5-Eu1-O3	127.6(1)	O2a-Eu1-O3	91.5(1)	O6b-Eu1-O3	78.1(1)		
O1-Eu1-O3	99.6(2)	O7-Eu1-O3	160.0(2)	O8-Eu1-O3	78.1(2)		
O5-Eu1-O4	76.7(1)	O2a-Eu1-O4	76.0(2)	O6a-Eu1-O4	121.8(2)		
2							
Tb1-O5	2.310(4)	Tb1-O2b	2.323(4)	Tb1-O6b	2.329(4)	Tb1-O1	2.360(4)
Tb1-O7	2.368(4)	Tb1-O8	2.385(5)	Tb1-O3	2.462(4)	Tb1-O4	2.476(4)
O5-Tb1-O2a	83.7(2)	O5-Tb1-O6b	149.3(2)	O2a-Tb1-O6b	77.6(2)		
O5-Tb1-O1	111.7(2)	O2a-Tb1-O1	148.6(2)	O6b-Tb1-O1	76.0(2)		
O5-Tb1-O7	70.6(1)	O2a-Tb1-O7	82.0(2)	O6b-Tb1-O7	82.7(2)		
O1-Tb1-O7	78.1(2)	O5-Tb1-O8	77.0(2)	O2a-Tb1-O8	145.6(2)		
O6b-Tb1-O8	130.4(2)	O1-Tb1-O8	65.8(2)	O7-Tb1-O8	116.9(2)		
O5-Tb1-O3	128.0(1)	O2a-Tb1-O3	91.8(2)	O6b-Tb1-O3	77.2(2)		
O1-Tb1-O3	98.6(2)	O7-Tb1-O3	159.8(2)	O8-Tb1-O3	78.5(2)		
O5-Tb1-O4	76.4(1)	O2a-Tb1-O4	75.8(2)	O6a-Tb1-O4	121.2(2)		

Symmetry code: a : -x+3/2, y-1/2, -z+3/2 b: -x+3/2, y+1/2, -z+3/2

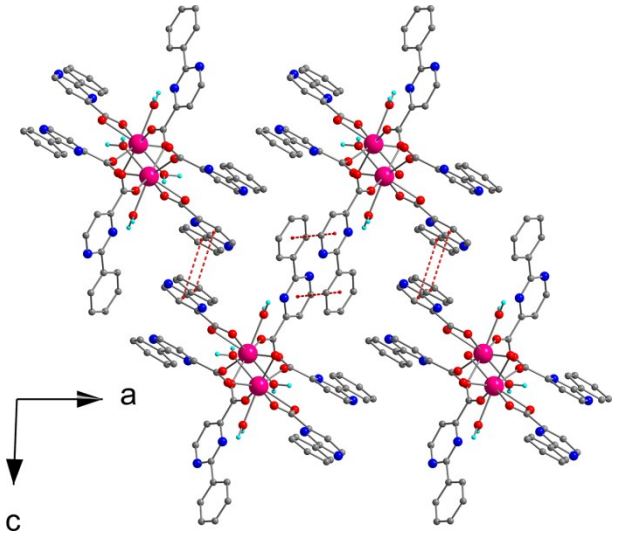
Table S2 Selected Bond Lengths (Å) and Bond Angles (deg) for compounds **3-5**.

3							
Eu-O3	2.330(2)	Eu-O2a	2.348(2)	Eu-O4b	2.360(1)	Eu-O5	2.378(2)
Eu-O7	2.429(2)	Eu-O1	2.440(2)	Eu-O6b	2.451(2)	Eu-O8	2.546(2)
O3-Eu-O2a	85.80(8)	O3-Eu-O4b	122.91(7)	O2a-Eu-O4b	131.50(8)		
O3-Eu-O5	77.32(7)	O2a-Eu-O5	73.39(7)	O4b-Eu-O5	144.50(7)		
O3-Eu-O7	140.38(8)	O2a-Eu-O7	103.51(8)	O4b-Eu-O7	79.30(7)		
O5-Eu-O7	69.08(7)	O3-Eu-O1	74.08(8)	O2a-Eu-O1	74.88(8)		
O4b-Eu-O1	77.14(8)	O5-Eu-O1	138.34(7)	O7-Eu-O1	145.52(7)		
O3-Eu-O6b	75.77(8)	O2a-Eu-O6b	148.54(7)	O4b-Eu-O6b	79.87(7)		
O5-Eu-O6b	77.77(7)	O7-Eu-O6b	77.09(7)	O1-Eu-O6b	122.33(7)		
O3-Eu-O8	144.09(9)	O2a-Eu-O8	67.56(8)	O4a-Eu-O8	67.67(8)		
O5-Eu-O8	114.78(7)	O7-Eu-O8	71.98(8)	O1-Eu-O8	75.93(8)		
O6b-Eu-O8	138.36(8)						
4							
Gd-O3	2.324(2)	Gd-O2a	2.339(3)	Gd-O4b	2.339(3)	Gd-O5	2.372(2)
Gd-O7	2.420(2)	Gd-O1	2.429(3)	Gd-O6b	2.445(2)	Gd-O8	2.535(3)
O3-Gd-O2a	85.7(1)	O3-Gd-O4b	85.7(1)	O2a-Gd-O4b	131.83(9)		
O3-Gd-O5	77.38(9)	O2a-Gd-O5	73.27(9)	O4b-Gd-O5	144.46(9)		
O3-Gd-O7	140.5(1)	O2a-Gd-O7	103.60(9)	O4b-Gd-O7	79.26(9)		
O5-Gd-O7	69.15(8)	O3-Gd-O1	74.0(1)	O2a-Gd-O1	75.17(9)		
O4b-Gd-O1	77.02(9)	O5-Gd-O1	138.50(9)	O7-Gd-O1	145.49(9)		
O3-Gd-O6b	75.59(9)	O2a-Gd-O6b	148.30(9)	O4b-Gd-O6b	79.80(9)		
O5-Gd-O6b	77.77(8)	O7-Gd-O6b	77.27(8)	O1-Gd-O6b	77.27(8)		
O3-Gd-O8	144.0(1)	O2a-Gd-O8	67.7(1)	O4a-Gd-O8	67.85(9)		
O5-Gd-O8	114.82(9)	O7-Gd-O8	72.0(1)	O1-Gd-O8	76.0(1)		
O6b-Gd-O8	138.59(9)						
5							
Tb-O3	2.300(2)	Tb-O2a	2.318(2)	Tb-O4b	2.331(2)	Tb-O5	2.350(2)
Tb-O7	2.398(2)	Tb-O1	2.411(2)	Tb-O6b	2.417(2)	Tb-O8	2.510(3)
O3-Tb-O2a	85.23(9)	O3-Tb-O4b	122.41(8)	O2a-Tb-O4b	132.28(9)		
O3-Tb-O5	77.45(8)	O2a-Tb-O5	73.55(8)	O4b-Tb-O5	144.25(8)		
O3-Tb-O7	140.71(9)	O2a-Tb-O7	104.08(9)	O4b-Tb-O7	79.22(8)		
O5-Tb-O7	69.25(8)	O3-Tb-O1	73.80(9)	O2a-Tb-O1	75.05(9)		
O4b-Tb-O1	77.02(9)	O5-Tb-O1	138.68(8)	O7-Tb-O1	145.44(8)		
O3-Tb-O6b	75.74(8)	O2a-Tb-O6b	148.63(8)	O4b-Tb-O6b	79.06(8)		
O5-Tb-O6b	78.06(8)	O7-Tb-O6b	77.46(8)	O1-Tb-O6b	121.43(8)		
O3-Tb-O8	143.90(9)	O2a-Tb-O8	67.93(9)	O4a-Tb-O8	68.28(9)		
O5-Tb-O8	114.87(8)	O7-Tb-O8	71.90(9)	O1-Tb-O8	76.15(9)		
O6b-Tb-O8	138.43(9)						

Symmetry code: a: x,-y+1/2,z+1/2 b : x,-y+1/2,z-1/2

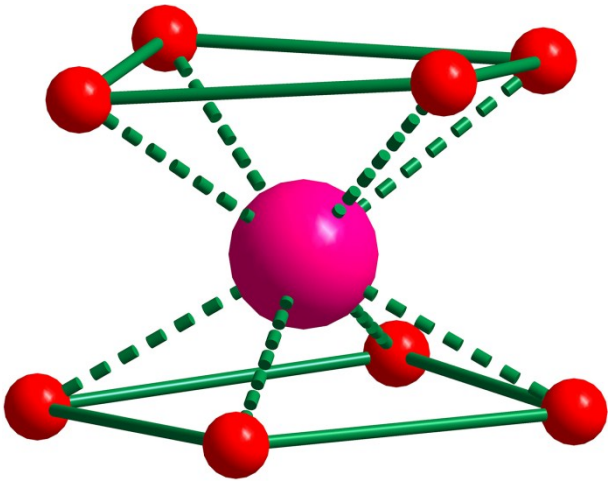


(a)

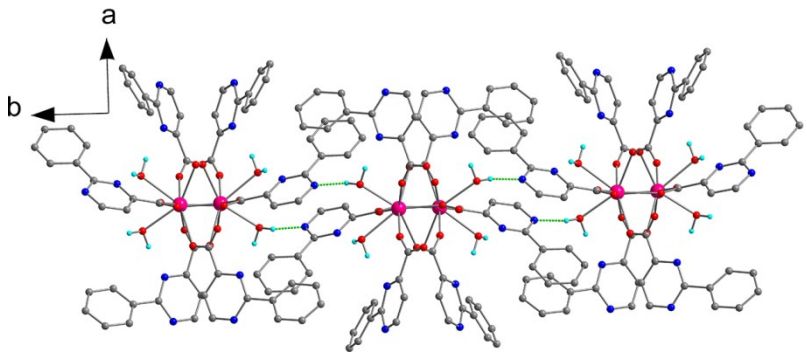


(b)

Fig. S1 The coordination polyhedron of Eu^{3+} (a), the 3D structure constructed by π-π stacking between the $ppmc^-$ ligands (b) in **1** (The hydrogen atoms are omitted for clarity).



(a)



(b)

Fig. S2 The coordination polyhedron of Eu^{3+} (a), the 2D structure (b) connected by hydrogen bonds in **3** (The hydrogen atoms are omitted for clarity).

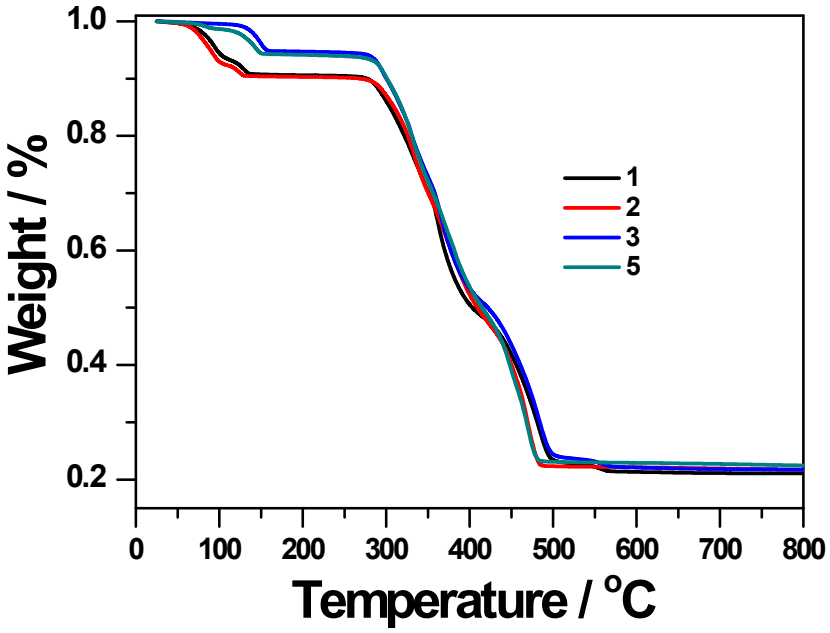


Fig. S3 TGA curve of complexes **1**, **2**, **3** and **5**.

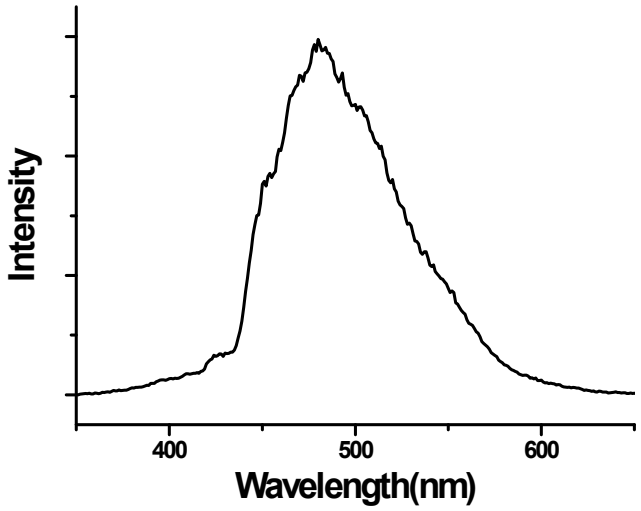
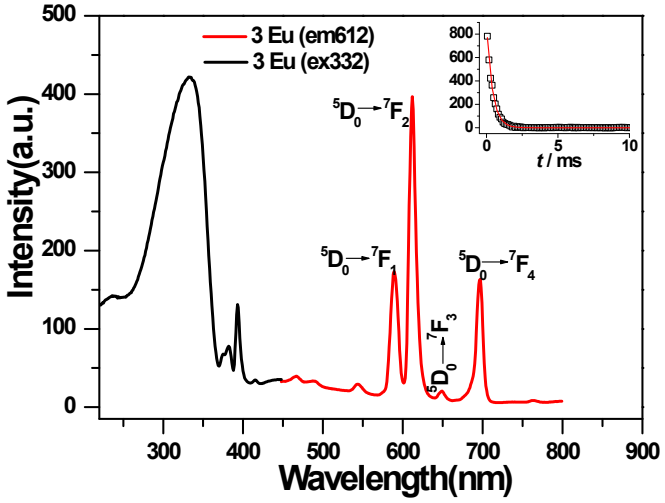
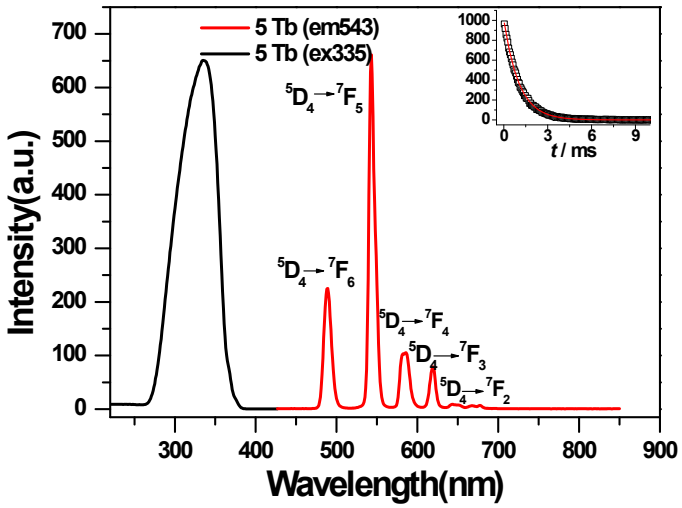


Fig. S4 Phosphorescence spectra of **4** at 77 K.

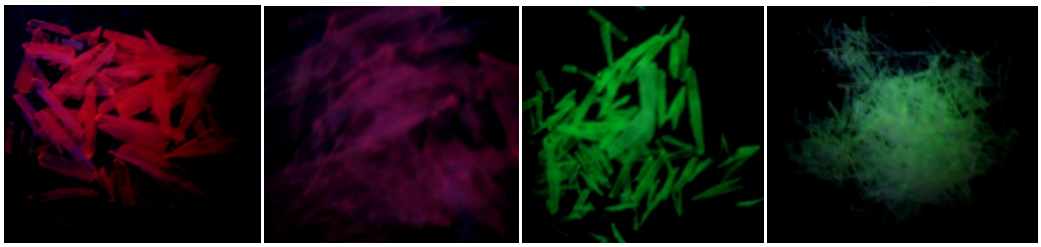


(a)



(b)

Fig. S5 Solid-state excitation/emission spectra and emission decay patterns (insets) of **3** (a) and **5** (b).



1 **3** **2** **5**

Fig. S6 Photos of compounds **1**, **2**, **3** and **5** under UV light.