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Luminescent Lanthanide-2-phenylpyrimidine-carboxylate Framework: Structure and Luminescence Tuning

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Table S1 Selected bond lengths (Å) and bond angles (deg) for compounds **1-2.**

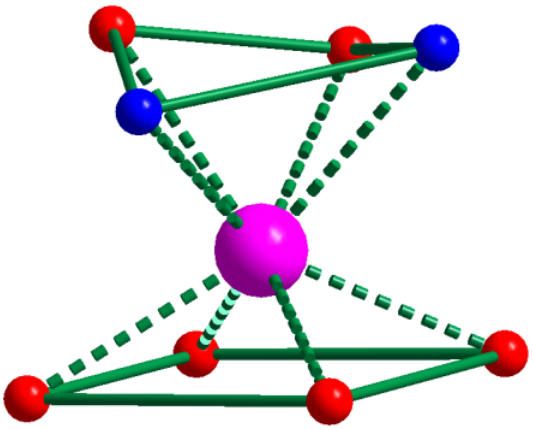
1							
Eu-O1	2.346(5)	Eu-O2a	2.337(5)	Eu-O3	2.380(5)	Eu-O4a	2.329(5)
Eu-O5	2.515(5)	Eu-O6	2.412(5)	Eu-N7	2.570(5)	Eu-N8	2.596(6)
O4a-Eu-O2a	80.1(2)	O4a-Eu-O1	77.5(2)	O2a-Eu-O1	124.7(2)		
O4a-Eu-O3	125.1(2)	O2a- Eu-O3	74.8(2)	O1-Eu-O3	78.2(2)		
O4a- Eu-O6	131.8(2)	O2a-Eu-O6	82.1(2)	O1-Eu-O6	146.4(2)		
O3-Eu-O6	91.9(2)	O4a-Eu-O5	79.5(2)	O2a-Eu-O5	74.0(2)		
O1-Eu-O5	146.5(2)	O3-Eu-O5	135.2(2)	O6-Eu-O5	52.6(2)		
O4a-Eu-N7	82.3(2)	O2a-Eu-N7	143.9(2)	O1-Eu-N7	81.1(2)		
O3-Eu-N7	140.0(2)	O6-Eu-N7	86.7(2)	O5-Eu-N7	72.0(2)		
O4a-Eu-N8	137.1(2)	O2a-Eu-N8	142.7(2)	O1-Eu-N8	72.7(2)		
O3-Eu-N8	77.9(2)	O6-Eu-N8	73.9(2)	O5-Eu-N8	110.5(2)		
N7-Eu-N8	63.3(2)						
2							
Tb-O1	2.329(3)	Tb-O2a	2.327(3)	Tb-O3	2.353(3)	Tb-O4a	2.296(3)
Tb-O5	2.505(3)	Tb-O6	2.399(3)	Tb-N7	2.554(3)	Tb-N8	2.586(3)
O4a-Tb-O2a	80.7(1)	O4a-Tb-O1	77.1(1)	O2a-Tb-O1	124.9(1)		
O4a-Tb-O3	125.4(1)	O2a-Tb-O3	74.4(1)	O1-Tb-O3	78.8(1)		
O4a-Tb-O6	132.3(1)	O2a-Tb-O6	81.5(1)	O1-Tb-O6	146.4(1)		
O3-Tb-O6	91.1(1)	O4a-Tb-O5	79.5(1)	O2a-Tb-O5	73.6(1)		
O1-Tb-O5	146.6(1)	O3-Tb-O5	134.6(1)	O6-Tb-O5	53.0(1)		
O4a-Tb-N7	81.6(1)	O2a-Tb-N7	143.7(1)	O1-Tb-N7	81.0(1)		
O3-Tb-N7	140.6(1)	O6-Tb-N7	87.5(1)	O5-Tb-N7	72.2(1)		
O4a-Tb-N8	136.7(1)	O2a-Tb-N8	142.4(1)	O1-Tb-N8	72.6(1)		
O3-Tb-N8	77.9(1)	O6-Tb-N8	74.0(1)	O5-Tb-N8	111.0(1)		
N7-Tb-N8	63.9(1)						

Table S2 Selected Bond Lengths (Å) and Bond Angles (deg) forCompounds **3-4**

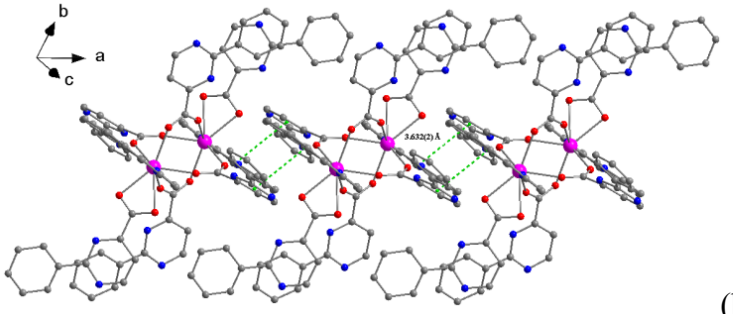
			3		
Eu-O1	2.300(3)	Eu-O3	2.389(3)	Eu-O5	2.399(2)
Eu-O7	2.443(3)	Eu-O6	2.420(2)	Eu-O4a	2.376(3)
Eu-N1	2.552(3)	Eu-N2	2.590(3)		
O1-Eu-O4a	149.9(1)	O1-Eu-O5	82.4(1)	O4a-Eu-O5	78.31(9)
O1-Eu-O3	85.5(1)	O4a-Eu-O3	110.77(9)	O5-Eu-O3	74.28(9)
O1-Eu-O6	74.98(9)	O4a-Eu-O6	76.39(9)	O5-Eu-O6	67.58(8)
O3-Eu-O6	138.89(9)	O1-Eu-O7	138.0(1)	O4a-Eu-O7	71.7(1)
O5-Eu-O7	128.21(9)	O3-Eu-O7	78.2(1)	O6-Eu-O7	138.6(1)
O1-Eu-N1	94.3(1)	O4a-Eu-N1	87.6(1)	O5-Eu-N1	142.94(9)
O3-Eu-N1	142.5(1)	O6-Eu-N1	75.86(9)	O7-Eu-N1	77.2(1)
O1-Eu-N2	71.1(1)	O4a-Eu-N2	134.8(1)		
			4		
Tb-O1	2.272(3)	Tb-O3	2.353(3)	Tb-O5	2.372(3)
Tb-O7	2.412(3)	Tb-O6	2.390(3)	Tb-O4a	2.344(3)
Tb-N1	2.528(3)	Tb-N2	2.569(3)		
O1-Tb-O4a	149.8(1)	O1-Tb-O5	82.5(1)	O4a-Tb-O5	78.4(1)
O1-Tb-O3	85.8(1)	O4a-Tb-O3	110.7(1)	O5-Tb-O3	74.11(9)
O1-Tb-O6	75.1(1)	O4a-Tb-O6	76.2(1)	O5-Tb-O6	67.92(9)
O3-Tb-O6	139.14(9)	O1-Tb-O7	137.9(1)	O4a-Tb-O7	71.8(1)
O5-Tb-O7	127.9(1)	O3-Tb-O7	77.8(1)	O6-Tb-O7	138.7(1)
O1-Tb-N1	94.6(1)	O4a-Tb-N1	86.9(1)	O5-Tb-N1	142.8(1)
O3-Tb-N1	142.9(1)	O6-Tb-N1	75.5(1)	O7-Tb-N1	77.3(1)
O1-Tb-N2	71.2(1)	O4a-Tb-N2	134.8(1)		

Table S3 Selected Bond Lengths (Å) and Bond Angles (deg) forCompounds **5-6**

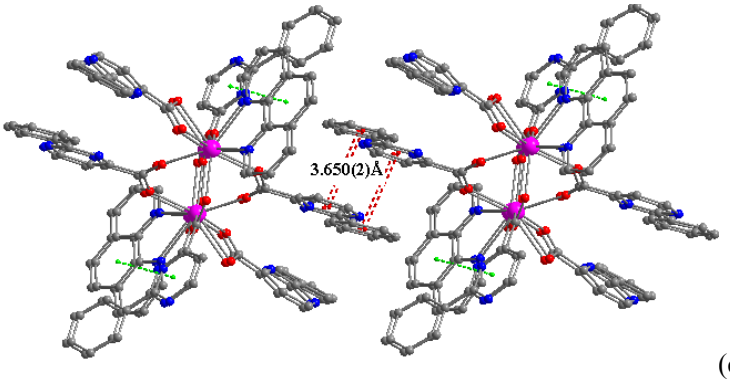
			5		
Eu-O1	2.404(3)	Eu-O2c	2.406(3)	Eu-O3a	2.505(3)
Eu-O4a	2.775(3)	Eu-O4d	2.409(3)	Eu-O5	2.451(3)
Eu-O6b	2.397(3)	Eu-N3	2.625(3)	Eu-N4	2.571(3)
O1-Eu-O6b	82.13(9)	O1-Eu-O2c	133.12(9)	O6b-Eu-O2c	141.48(9)
O1-Eu-O5	137.28(9)	O6b-Eu-O5	67.13(9)	O2c- Eu-O5	74.81(9)
O1-Eu-O4d	74.8(1)	O6b-Eu-O4d	143.6(1)	O2c-Eu-O4d	72.0(1)
O5-Eu-O4d	145.63(9)	O1-Eu-O3a	74.1(1)	O6b-Eu-O3a	77.3(1)
O2c-Eu-O3a	96.1(1)	O5-Eu-O3a	70.8(1)	O4d-Eu-O3a	121.1(1)
O1-Eu-N4	137.9(1)	O6b-Eu-N4	89.8(1)	O2c-Eu-N4	73.4(1)
O5-Eu-N4	73.2(1)	O4d-Eu-N4	88.9(1)	O3a-Eu-N4	144.0(1)
O1-Eu-N3	75.0(1)	O6b-Eu-N3	72.3(1)	O2c-Eu-N3	124.9(1)
O5-Eu-N3	119.2(1)	O4d-Eu-N3	74.8(1)		
			6		
Tb-O1	2.437(2)	Tb-O2	2.439(2)	Tb-O3a	2.306(2)
Tb-O4d	2.351(2)	Tb-O5	2.304(2)	Tb-O6c	2.335(2)
Tb-N3	2.563(3)	Tb-N4	2.567(3)		
O5-Tb-O3a	77.29(8)	O5-Tb-O6c	124.72(8)	O3a-Tb-O6c	79.88(7)
O6c-Tb-O4d	75.13(7)	O5-Tb-O4d	78.48(8)	O3a-Tb-O4d	125.29(7)
O5-Tb-O1	78.44(8)	O3a-Tb-O1	81.58(7)	O6c-Tb-O1	145.47(7)
O4d-Tb-O1	138.76(7)	O5-Tb-O2	79.63(8)	O3a-Tb-O2	132.77(7)
O6c-Tb-O2	145.74(7)	O4d-Tb-O2	88.84(7)	O1-Tb-O2	53.58(7)
O5-Tb-N3	143.53(9)	O3a-Tb-N3	139.18(9)	O6c-Tb-N3	73.77(8)
O4d-Tb-N3	77.12(8)	O1-Tb-N3	103.28(8)	O2-Tb-N3	73.21(8)
O5-Tb-N4	146.68(9)	O3a-Tb-N4	78.71(9)	O6c-Tb-N4	72.51(8)
O4d-Tb-N4	134.71(9)	O1-Tb-N4	75.45(8)	O2-Tb-N4	100.62(8)
N3-Tb-N4	64.01(9)				



(a)

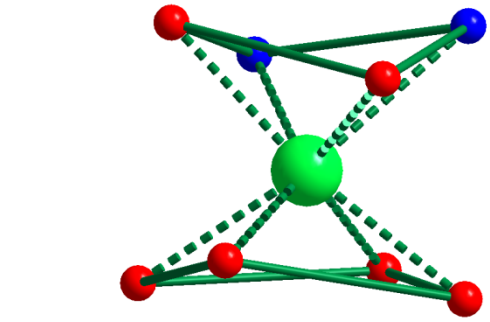


(b)

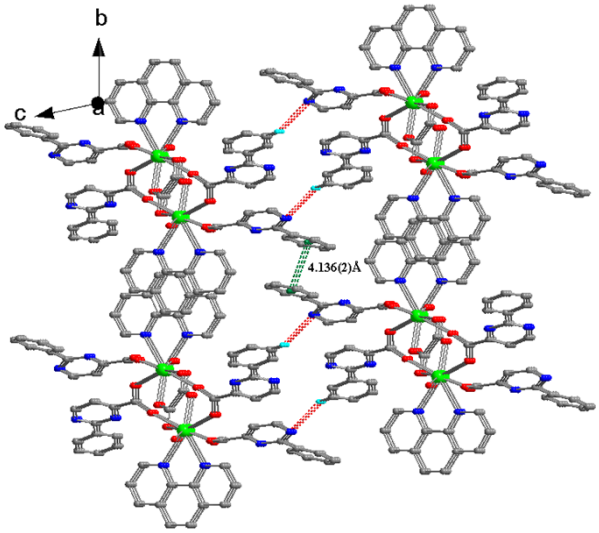


(c)

Fig. S1 The coordination polyhedron of Ln^{3+} (a), the 1D chain structure (b) and the 3D structure (c) constructed by π-π stacking between the phen and $ppmc^-$ ligands in **1** and **2**. (phen and the hydrogen atoms of ring were omitted for clarity)

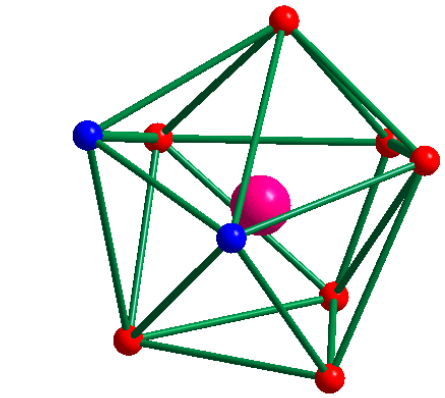


(a)

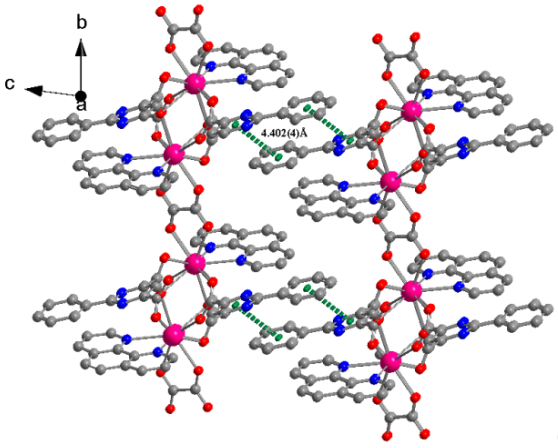


(b)

Fig. S2 The coordination polyhedron of Ln^{3+} (a) the 3D structure constructed by π-π stacking and the C-H···N weak hydrogen bonds between the phen and $ppmc^{-}$ ligands (b) in **3** and **4**.

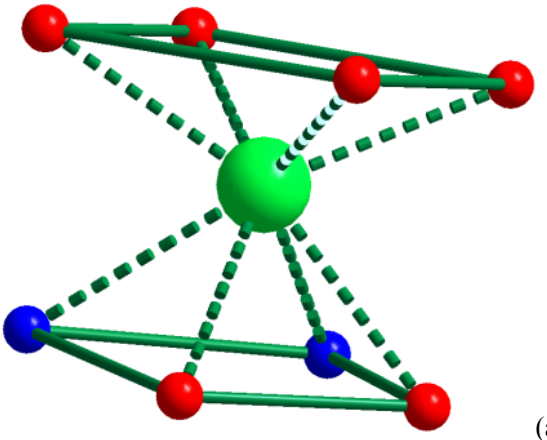


(a)

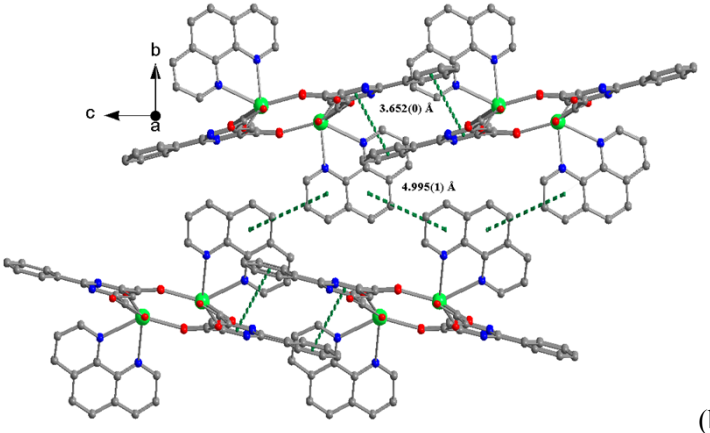


(b)

Fig. S3 The coordination polyhedron of Eu^{3+} (a) and the 3D supramolecular structure connected by π-π stacking (b) in **5**.



(a)



(b)

Fig. S4 The coordination polyhedron of Tb^{3+} (a) and the 3D supramolecular structure connected by π-π stacking (b) in **6**.

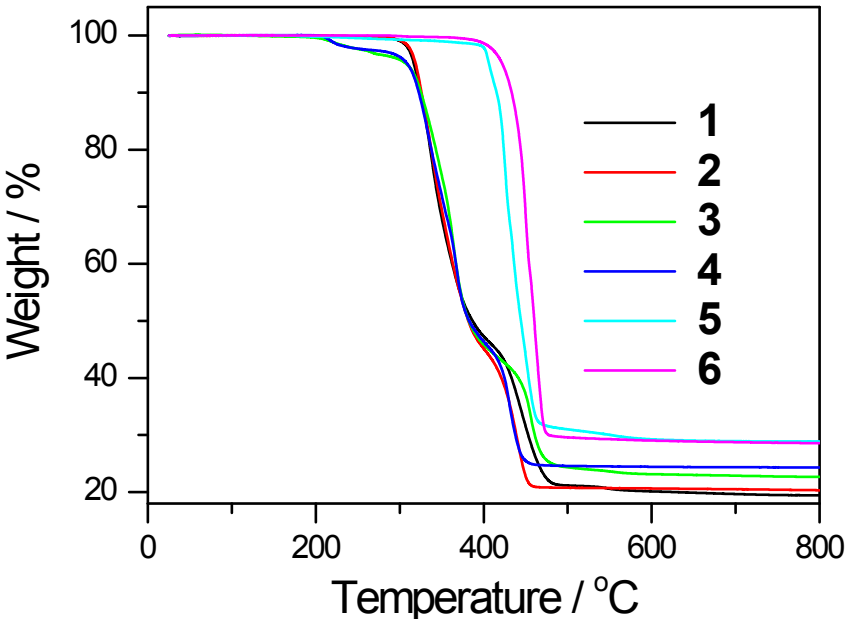
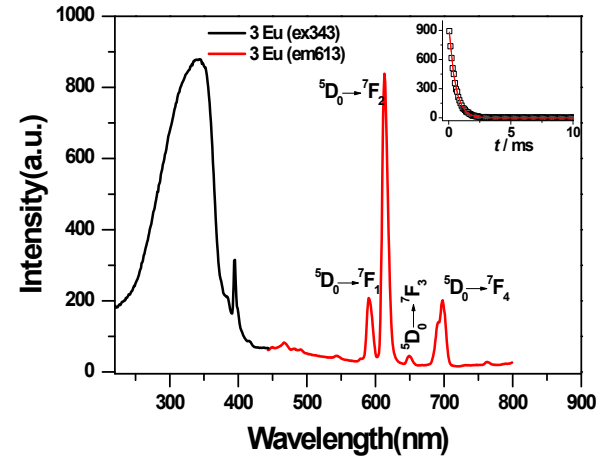
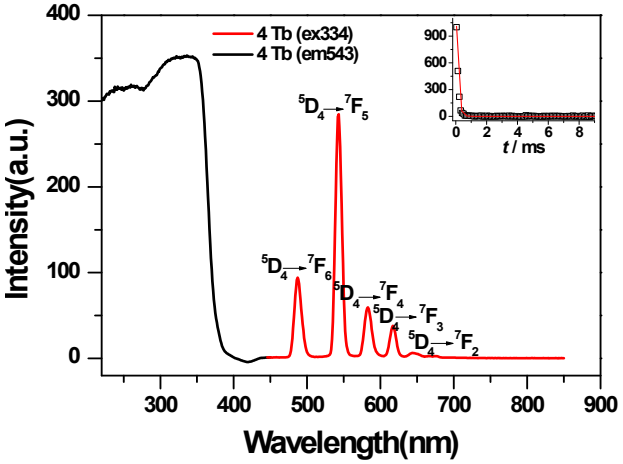


Fig. S5 TGA curve of complexes **1**-**6**.

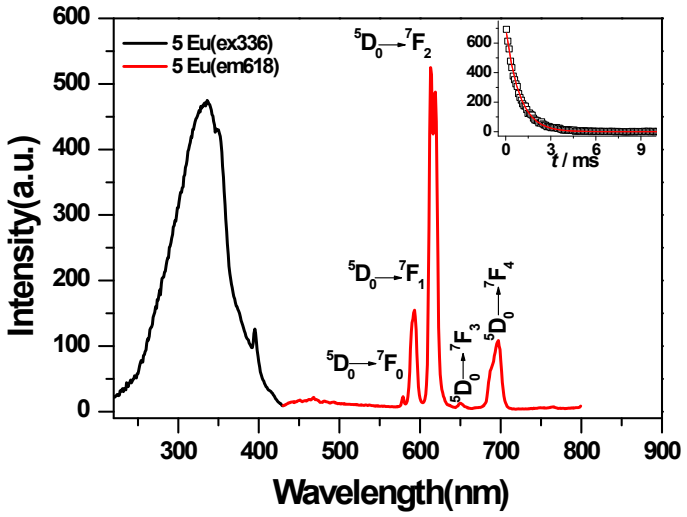


(a)

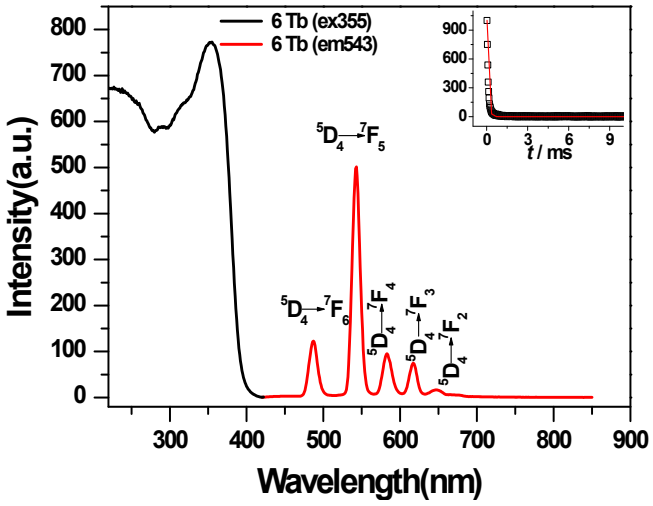


(b)

Fig. S6 Solid-state excitation/emission spectra and the emission decay pattern (inset) of **3** (a) and **4** (b).



(a)



(b)

Fig. S7 Solid-state excitation/emission spectra and the emission decay pattern (inset) of **5** (a) and **6** (b).

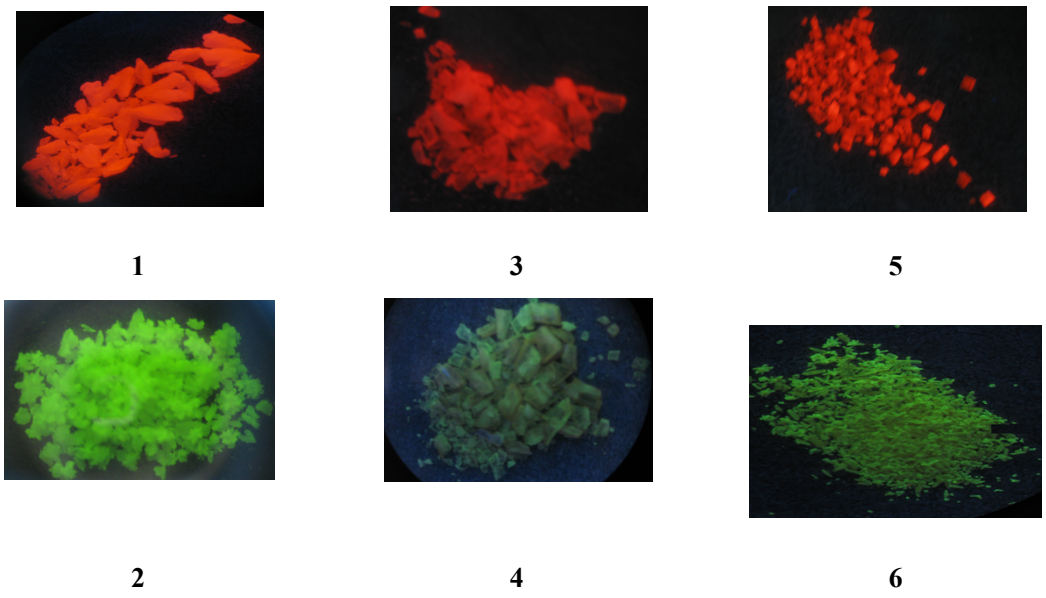


Fig. S8 Photos of compound **1-6** under UV light.