Electronic Supplementary Material (ESI) for CrystEngComm.

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Self-assembly synthesis, structural features, reversible temperature-induced dehydration/hydration, magnetic and luminescent properties of lanthanide(III) compounds derived from 5-fluoronicotinic acid

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Electronic Supplementary Information contains: selected bonding (Table S1) and H-bonding (Table S2) parameters, thermal analysis data (Table S3), additional luminescent data (Table S4), TGA curves (Fig. S1), PXRD patterns (Figs. S2–S5), UV-Vis absorption spectra (Fig. S6) and emission spectra (Figs. S7–S9) for the obtained compounds.

Table S1 Selected bond lengths [Å] and angles [°] for the compounds **1**–**8**.[a]

1					
La(1)-O(1)	2.754(4)	La(1)-O(2)	2.622(4)	La(1)-O(3)	2.604(4)
La(1)-O(4)	2.569(3)	La(1)-O(5)	2.427(3)	La(1)-O(6)#1	2.453(3)
La(1)-O(7)	2.556(3)	La(1)-O(8)	2.526(3)	La(1)-O(9)	2.535(3)
O(5)-La(1)-O(6)#1	83.70(11)	O(5)-La(1)-O(8)	135.56(11)	O(6)#1-La(1)-O(8)	140.71(11)
O(5)-La(1)-O(9)	144.27(13)	O(6)#1-La(1)-O(9)	73.04(11)	O(8)-La(1)-O(9)	71.28(11)
O(5)-La(1)-O(7)	68.88(12)	O(6)#1-La(1)-O(7)	141.66(11)	O(8)-La(1)-O(7)	71.73(11)
O(9)-La(1)-O(7)	143.00(12)	O(5)-La(1)-O(4)	83.50(12)	O(6)#1-La(1)-O(4)	122.00(12)
O(8)-La(1)-O(4)	71.40(12)	O(9)-La(1)-O(4)	86.27(12)	O(7)-La(1)-O(4)	82.09(12)
O(5)-La(1)-O(3)	75.47(12)	O(6)#1-La(1)-O(3)	71.57(11)	O(8)-La(1)-O(3)	111.24(12)
O(9)-La(1)-O(3)	71.66(12)	O(7)-La(1)-O(3)	123.07(12)	O(4)-La(1)-O(3)	50.45(10)
O(5)-La(1)-O(2)	131.29(12)	O(6)#1-La(1)-O(2)	87.24(12)	O(8)-La(1)-O(2)	68.27(11)
O(9)-La(1)-O(2)	75.20(12)	O(7)-La(1)-O(2)	91.20(12)	O(4)-La(1)-O(2)	139.16(12)
O(3)-La(1)-O(2)	144.59(11)	O(5)-La(1)-O(1)	84.07(11)	O(6)#1-La(1)-O(1)	70.05(11)
O(8)-La(1)-O(1)	109.05(12)	O(9)-La(1)-O(1)	111.71(11)	O(7)-La(1)-O(1)	80.59(11)
O(4)-La(1)-O(1)	161.43(10)	O(3)-La(1)-O(1)	138.03(11)	O(2)-La(1)-O(1)	48.14(10)
2					
Pr(1)-O(1)	2.585(4)	Pr(1)-O(2)	2.527(3)	Pr(1)-O(3)	2.731(4)
Pr(1)-O(4)	2.579(4)	Pr(1)-O(5)	2.416(4)	Pr(1)-O(6)#1	2.388(4)
Pr(1)-O(7)	2.482(4)	Pr(1)-O(8)	2.507(4)	Pr(1)-O(9)	2.497(4)
O(6)#1-Pr(1)-O(5)	83.52(13)	O(6)#1-Pr(1)-O(7)	135.99(13)	O(5)-Pr(1)-O(7)	140.47(13)
O(6)#1-Pr(1)-O(9)	144.21(14)	O(5)-Pr(1)-O(9)	73.38(14)	O(7)-Pr(1)-O(9)	70.82(15)
O(6)#1-Pr(1)-O(8)	69.42(14)	O(5)-Pr(1)-O(8)	140.70(14)	O(7)-Pr(1)-O(8)	72.14(15)
O(9)-Pr(1)-O(8)	142.95(15)	O(6)#1-Pr(1)-O(2)	84.00(14)	O(5)-Pr(1)-O(2)	122.64(12)
O(7)-Pr(1)-O(2)	70.92(13)	O(9)-Pr(1)-O(2)	85.91(14)	O(8)-Pr(1)-O(2)	83.33(13)
O(6)#1-Pr(1)-O(4)	131.08(14)	O(5)-Pr(1)-O(4)	86.87(13)	O(7)-Pr(1)-O(4)	68.44(13)
O(9)-Pr(1)-O(4)	75.38(14)	O(8)-Pr(1)-O(4)	90.00(14)	O(2)-Pr(1)-O(4)	138.90(14)
O(6)#1-Pr(1)-O(1)	75.66(14)	O(5)-Pr(1)-O(1)	71.64(12)	O(7)-Pr(1)-O(1)	111.10(13)
O(9)-Pr(1)-O(1)	71.35(13)	O(8)-Pr(1)-O(1)	124.69(12)	O(2)-Pr(1)-O(1)	51.02(12)
O(4)-Pr(1)-O(1)	144.30(14)	O(6)#1-Pr(1)-O(3)	83.20(13)	O(5)-Pr(1)-O(3)	70.18(13)
O(7)-Pr(1)-O(3)	109.38(13)	O(9)-Pr(1)-O(3)	112.83(12)	O(8)-Pr(1)-O(3)	78.54(13)
O(2)-Pr(1)-O(3)	160.59(13)	O(4)-Pr(1)-O(3)	48.65(13)	O(1)-Pr(1)-O(3)	137.96(13)
3					
Nd(1)-O(1)	2.571(3)	Nd(1)-O(2)	2.507(3)	Nd(1)-O(3)	2.720(3)
Nd(1)-O(4)	2.564(3)	Nd(1)-O(5)	2.369(3)	Nd(1)-O(6)#1	2.396(3)
Nd(1)-O(7)	2.485(3)	Nd(1)-O(8)	2.473(3)	Nd(1)-O(9)	2.471(3)
O(5)-Nd(1)-O(6)#1	83.47(12)	O(5)-Nd(1)-O(9)	144.22(11)	O(6)#1-Nd(1)-O(9)	73.54(12)
O(5)-Nd(1)-O(8)	136.05(13)	O(6)#1-Nd(1)-O(8)	140.46(12)	O(9)-Nd(1)-O(8)	70.79(13)
O(5)-Nd(1)-O(7)	69.61(12)	O(6)#1-Nd(1)-O(7)	140.29(12)	O(9)-Nd(1)-O(7)	142.90(12)
O(8)-Nd(1)-O(7)	72.15(13)	O(5)-Nd(1)-O(2)	83.98(12)	O(6)#1-Nd(1)-O(2)	122.93(10)
O(9)-Nd(1)-O(2)	85.97(12)	O(8)-Nd(1)-O(2)	70.98(11)	O(7)-Nd(1)-O(2)	83.68(12)
O(5)-Nd(1)-O(4)	131.11(12)	O(6)#1-Nd(1)-O(4)	86.34(11)	O(9)-Nd(1)-O(4)	75.17(12)
O(8)-Nd(1)-O(4)	68.63(11)	O(7)-Nd(1)-O(4)	89.94(12)	O(2)-Nd(1)-O(4)	139.11(12)
O(5)-Nd(1)-O(1)	75.40(12)	O(6)#1-Nd(1)-O(1)	71.80(11)	O(9)-Nd(1)-O(1)	71.59(11)
O(8)-Nd(1)-O(1)	111.37(11)	O(7)-Nd(1)-O(1)	125.03(11)	O(2)-Nd(1)-O(1)	51.16(11)
O(4)-Nd(1)-O(1)	144.15(12)	O(5)-Nd(1)-O(3)	82.80(11)	O(6)#1-Nd(1)-O(3)	69.85(11)

O(9)-Nd(1)-O(3)	113.13(11)	O(8)-Nd(1)-O(3)	109.64(11)	O(7)-Nd(1)-O(3)	78.05(11)
O(2)-Nd(1)-O(3)	160.30(12)	O(4)-Nd(1)-O(3)	48.99(11)	O(1)-Nd(1)-O(3)	137.55(11)
4					
Eu(1)-O(1)	2.720(4)	Eu(1)-O(2)	2.509(3)	Eu(1)-O(3)	2.556(3)
Eu(1)-O(4)	2.458(3)	Eu(1)-O(5)	2.326(3)	Eu(1)-O(6)#1	2.356(3)
Eu(1)-O(7)	2.444(3)	Eu(1)-O(8)	2.443(3)	Eu(1)-O(9)	2.439(3)
O(5)-Eu(1)-O(6)#1	83.02(11)	O(5)-Eu(1)-O(9)	144.21(10)	O(6)#1-Eu(1)-O(9	73.34(11)
O(5)-Eu(1)-O(8)	135.95(11)	O(6)#1-Eu(1)-O(8)	141.03(11	O(9)-Eu(1)-O(8)	71.74(11)
O(5)-Eu(1)-O(7)	70.18(10)	O(6)#1-Eu(1)-O(7)	140.27(11)	O(9)-Eu(1)-O(7)	142.79(11)
O(8)-Eu(1)-O(7)	71.11(11)	O(5)-Eu(1)-O(4)	84.07(11)	O(6)#1-Eu(1)-O(4)	123.86(10)
O(9)-Eu(1)-O(4)	87.20(11)	O(8)-Eu(1)-O(4)	71.02(11)	O(7)-Eu(1)-O(4)	82.88(11)
O(5)-Eu(1)-O(2)	130.58(11)	O(6)#1-Eu(1)-O(2)	85.99(11)	O(9)-Eu(1)-O(2)	74.92(11)
O(8)-Eu(1)-O(2)	68.73(11)	O(7)-Eu(1)-O(2)	89.72(11)	O(4)-Eu(1)-O(2)	139.30(11)
O(5)-Eu(1)-O(3)	75.78(10)	O(6)#1-Eu(1)-O(3)	71.76(10)	O(9)-Eu(1)-O(3)	71.53(11)
O(8)-Eu(1)-O(3)	112.00(11)	O(7)-Eu(1)-O(3)	125.64(11)	O(4)-Eu(1)-O(3)	52.11(10)
O(2)-Eu(1)-O(3)	143.78(11)	O(5)-Eu(1)-O(1)	81.59(11)	O(6)#1-Eu(1)-O(1)	69.63(10)
O(9)-Eu(1)-O(1)	113.40(11)	O(8)-Eu(1)-O(1)	109.69(10)	O(7)-Eu(1)-O(1)	77.67(11)
O(4)-Eu(1)-O(1)	158.85(10)	O(2)-Eu(1)-O(1)	49.58(10)	O(3)-Eu(1)-O(1)	137.06(10)
5					
Gd(1)-O(1)	2.446(3)	Gd(1)-O(2)	2.552(4)	Gd(1)-O(3)	2.491(3)
Gd(1)-O(4)	2.712(4)	Gd(1)-O(5)	2.340(3)	Gd(1)-O(6)#1	2.311(3)
Gd(1)-O(7)	2.423(3)	Gd(1)-O(8)	2.433(3)	Gd(1)-O(9)	2.428(4)
O(6)#1-Gd(1)-O(5)	82.92(11)	O(6)#1-Gd(1)-O(7)	144.05(13)	O(5)-Gd(1)-O(7)	73.51(11)
O(6)#1-Gd(1)-O(9)	70.47(12)	O(5)-Gd(1)-O(9)	140.02(12)	O(7)-Gd(1)-O(9)	142.69(12)
O(6)#1-Gd(1)-O(8)	135.80(12)	O(5)-Gd(1)-O(8)	141.27(11)	O(7)-Gd(1)-O(8)	71.79(13)
O(9)-Gd(1)-O(8)	70.98(12)	O(6)#1-Gd(1)-O(1)	84.18(12)	O(5)-Gd(1)-O(1)	124.09(12)
O(7)-Gd(1)-O(1)	86.98(12)	O(9)-Gd(1)-O(1)	83.20(13)	O(8)-Gd(1)-O(1)	70.58(12)
O(6)#1-Gd(1)-O(3)	130.44(12)	O(5)-Gd(1)-O(3)	85.70(12)	O(7)-Gd(1)-O(3)	75.15(12)
O(9)-Gd(1)-O(3)	89.41(13)	O(8)-Gd(1)-O(3)	69.29(11)	O(1)-Gd(1)-O(3)	139.41(11)
O(6)#1-Gd(1)-O(2)	75.77(12)	O(5)-Gd(1)-O(2)	71.78(11)	O(7)-Gd(1)-O(2)	71.30(12)
O(9)-Gd(1)-O(2)	126.16(11)	O(8)-Gd(1)-O(2)	111.80(12)	O(1)-Gd(1)-O(2)	52.31(11)
O(3)-Gd(1)-O(2)	143.63(12)	O(6)#1-Gd(1)-O(4)	81.28(11)	O(5)-Gd(1)-O(4)	69.67(12)
O(7)-Gd(1)-O(4)	113.97(11)	O(9)-Gd(1)-O(4)	77.05(12)	O(8)-Gd(1)-O(4)	110.05(12)
O(1)-Gd(1)-O(4)	158.49(12)	O(3)-Gd(1)-O(4)	49.69(10)	O(2)-Gd(1)-O(4)	137.00(11)
6					
Tb(1)-O(1)	2.555(3)	Tb(1)-O(2)	2.423(3)	Tb(1)-O(3)	2.739(3)
Tb(1)-O(4)	2.473(3)	Tb(1)-O(5)	2.319(3)	Tb(1)-O(6)#1	2.304(3)
Tb(1)-O(7)	2.404(3)	Tb(1)-O(8)	2.417(3)	Tb(1)-O(9)	2.413(3)
O(6)#1-Tb(1)-O(5)	82.89(10)	O(6)#1-Tb(1)-O(7)	143.94(10)	O(5)-Tb(1)-O(7)	74.01(10)
O(6)#1-Tb(1)-O(9)	70.72(10)	O(5)-Tb(1)-O(9)	138.98(10)	O(7)-Tb(1)-O(9)	142.67(10)
O(6)#1-Tb(1)-O(8)	136.61(11)	O(5)-Tb(1)-O(8)	140.49(11)	O(7)-Tb(1)-O(8)	70.56(11)
O(9)-Tb(1)-O(8)	72.27(11)	O(6)#1-Tb(1)-O(2)	83.66(10)	O(5)-Tb(1)-O(2)	124.27(9)
O(7)-Tb(1)-O(2)	86.89(11)	O(9)-Tb(1)-O(2)	84.24(11)	O(8)-Tb(1)-O(2)	70.83(10)
O(6)#1-Tb(1)-O(4)	130.13(10)	O(5)-Tb(1)-O(4)	85.64(10)	O(7)-Tb(1)-O(4)	75.94(11)
O(9)-Tb(1)-O(4)	88.03(11)	O(8)-Tb(1)-O(4)	69.40(10)	O(2)-Tb(1)-O(4)	139.97(10)
O(6)#1-Tb(1)-O(1)	75.82(10)	O(5)-Tb(1)-O(1)	71.96(10)	O(7)-Tb(1)-O(1)	70.93(11)
O(9)-Tb(1)-O(1)	127.39(11)	O(8)-Tb(1)-O(1)	111.13(10)	O(2)-Tb(1)-O(1)	52.31(10)
O(4)-Tb(1)-O(1)	143.90(11)	O(6)#1-Tb(1)-O(3)	81.22(10)	O(5)-Tb(1)-O(3)	69.48(10)
O(7)-Tb(1)-O(3)	114.59(11)	O(9)-Tb(1)-O(3)	75.75(10)	O(8)-Tb(1)-O(3)	110.57(10)

O(2)-Tb(1)-O(3)	158.01(10)	O(4)-Tb(1)-O(3)	49.45(10)	O(1)-Tb(1)-O(3)	137.00(10)
7					
Tm(1)-O(1)	2.378(4)	Tm(1)-O(2)	2.420(4)	Tm(1)-O(3)	2.259(4)
Tm(1)-O(4)#1	2.277(4)	Tm(1)-O(5)	2.359(4)	Tm(1)-O(6)	2.324(4)
Tm(1)-O(7)	2.333(4)	Tm(1)-O(8)	2.378(4)	O(3)-Tm(1)-O(4)#1	104.37(14)
O(3)-Tm(1)-O(6)	145.16(14)	O(4)#1-Tm(1)-O(6)	84.98(15)	O(3)-Tm(1)-O(7)	142.87(15)
O(4)#1-Tm(1)-O(7)	77.32(15)	O(6)-Tm(1)-O(7)	71.66(14)	O(3)-Tm(1)-O(5)	75.32(15)
O(4)#1-Tm(1)-O(5)	78.14(14)	O(6)-Tm(1)-O(5)	73.95(14)	O(7)-Tm(1)-O(5)	139.02(15)
O(3)-Tm(1)-O(1)	88.93(15)	O(4)#1-Tm(1)-O(1)	153.81(14)	O(6)-Tm(1)-O(1)	96.98(15)
O(7)-Tm(1)-O(1)	78.56(15)	O(5)-Tm(1)-O(1)	127.60(13)	O(3)-Tm(1)-O(8)	71.53(14)
O(4)#1-Tm(1)-O(8)	79.81(16)	O(6)-Tm(1)-O(8)	143.32(15)	O(7)-Tm(1)-O(8)	72.41(14)
O(5)-Tm(1)-O(8)	133.62(15)	O(1)-Tm(1)-O(8)	83.36(15)	O(3)-Tm(1)-O(2)	78.41(14)
O(4)#1-Tm(1)-O(2)	149.52(15)	O(6)-Tm(1)-O(2)	77.35(14)	O(7)-Tm(1)-O(2)	119.00(14)
O(5)-Tm(1)-O(2)	73.23(14)	O(1)-Tm(1)-O(2)	54.58(14)	O(8)-Tm(1)-O(2)	128.32(15)
8					
Eu(1)-O(1)	2.328(5)	Eu(1)-O(3)	2.292(4)	Eu(1)-O(5)	2.409(5)
Eu(1)-O(6)	2.515(5)	Eu(1)-O(7)	2.578(5)	Eu(1)-N(3)	2.636(5)
Eu(1)-N(4)	2.653(6)	Eu(1)-N(5)	2.714(6)	Eu(1)-N(6)	2.646(6)
O(3)-Eu(1)–O(1)	102.20(18)	O(1)-Eu(1)-O(5)	78.08(19)	O(3)-Eu(1)-O(6)	75.39(17)
O(1)-Eu(1)-O(6)	145.38(18)	O(5)-Eu(1)-O(6)	123.44(16)	O(3)-Eu(1)-O(7)	120.56(17)
O(1)-Eu(1)-O(7)	135.50(18)	O(5)-Eu(1)-O(7)	73.48(18)	O(6)-Eu(1)-O(7)	50.18(16)
O(3)-Eu(1)-N(3)	135.51(17)	O(1)-Eu(1)-N(3)	73.92(18)	O(5)-Eu(1)-N(3)	78.18(17)
O(6)-Eu(1)-N(3)	83.93(18)	O(7)-Eu(1)-N(3)	67.31(17)	O(3)-Eu(1)-N(6)	70.79(17)
O(1)-Eu(1)-N(6)	75.54(18)	O(5)-Eu(1)-N(6)	76.20(17)	O(6)-Eu(1)-N(6)	132.26(17)
O(7)-Eu(1)-N(6)	127.65(17)	N(3)-Eu(1)-N(6)	143.40(19)	O(3)-Eu(1)-N(4)	74.86(16)
O(1)-Eu(1)-N(4)	73.0(2)	O(5)-Eu(1)-N(4)	135.21(16)	O(6)-Eu(1)-N(4)	73.11(17)
O(7)-Eu(1)-N(4)	105.07(17)	N(3)-Eu(1)-N(4)	61.46(17)	N(6)-Eu(1)-N(4)	126.37(17)
O(3)-Eu(1)-N(5)	77.23(16)	O(1)-Eu(1)-N(5)	134.95(19)	O(5)-Eu(1)-N(5)	78.92(17)
O(6)-Eu(1)-N(5)	78.97(18)	O(7)-Eu(1)-N(5)	71.34(17)	N(3)-Eu(1)-N(5)	136.87(17)
N(6)-Eu(1)-N(5)	61.58(18)	N(4)-Eu(1)-N(5)	144.49(18)	O(3)-Eu(1)-O(5)	145.62(17)

[a] Symmetry transformations used to generate equivalent atoms: #1 $-x+1$, $-y$, $-z$ for **1**; #1 $-x+1$, $-y+1$, $-z$ for **2**; #1 $-x+1$, $-y$, $-z+1$ for **3**; #1 $-x$, $-y+1$, $-z+1$ for **4**; #1 $-x+2$, $-y$, $-z+1$ for **5**; #1 $-x+1$, $-y+1$, $-z+1$ for **6**; #1 $-x+1$, $-y$, $-z+1$ for **7**.

Table S2 Hydrogen bonds in crystal packing [Å, °] of **1**–**8**.

Complexes	D-H…A	d(D-H)	d(H…A)	d(D…A)	∠DHA	Symmetry code
1	O(7)-H(1W)···O(1)	0.85	2.08	2.839	147.9	$-x$, $-y+1$, $-z+1$
	O(8)-H(3W)···N(2)	0.85	2.07	2.740	135.2	$-x$, $-y+1$, $-z+2$
	O(8)-H(3W)···O(10)	0.85	1.97	2.816	179.2	$x-1$, y, z
	O(9)-H(5W)···N(1)	0.86	2.04	2.820	149.6	$-x$, $-y+2$, $-z+1$
	O(9)-H(6W)···O(10)	0.86	2.05	2.767	140.4	

	O(10)-H(7W)···N(3)	0.89	1.89	2.778	171	*x*, *y*+1, *z*
	O(10)-H(8W)···O(2)	0.83	2.14	2.805	137	*x*+1, *y*, *z*
2	O(7)-H(1W)···N(1)	0.88	2.03	2.746	136.9	-*x*, -*y*, -*z*+1
	O(7)-H(2W)···O(10)	0.88	2.06	2.821	143.2	*x*-1, *y*, *z*
	O(8)-H(3W)···O(1)	0.88	2.11	2.843	141.0	*x*-1, *y*, *z*
	O(8)-H(4W)···O(3)	0.88	2.21	2.836	128.4	-*x*, -*y*, -*z*
	O(9)-H(5W)···N(2)	0.89	2.00	2.810	151.2	-*x*, -*y*+1, -*z*
	O(9)-H(6W)···O(10)	0.89	2.03	2.771	140.7	
	O(10)-H(7W)···O(4)	0.85	2.05	2.805	147.7	*x*+1, *y*, *z*
	O(10)-H(8W)···N(3)	0.85	1.94	2.774	168.0	-*x*+1, -*y*+1, -*z*
3	O(10)-H(8W)···N(3)	0.85	1.94	2.780	167.5	*x*, *y*+1, *z*
	O(10)-H(7W)···O(4)	0.85	2.02	2.814	155.3	*x*+1, *y*, *z*
	O(9)-H(6W)···O(10)	0.90	1.98	2.772	144.9	
	O(9)-H(5W)···N(2)	0.91	2.00	2.822	151.2	-*x*, -*y*+2, -*z*
	O(8)-H(4W)···O(10)	0.87	2.10	2.810	137.5	*x*-1, *y*, *z*
	O(8)-H(3W)···N(1)	0.87	2.05	2.750	136.9	-*x*, -*y*+1, -*z*+1
	O(7)-H(1W)···O(3)	0.91	2.09	2.841	139.0	-*x*, -y+1, -*z*
	O(7)-H(2W)···O(1)	0.91	2.12	2.852	137.3	*x*-1, *y*, *z*
4	O(8)-H(4W)···N(2)	0.85	2.09	2.758	135.0	-*x*+1, -*y*+1, -*z*
	O(7)-H(2W)···O(1)	0.86	2.13	2.830	139.3	-*x*+1, -*y*+1, -*z*+1
	O(7)-H(1W)···O(3)	0.86	2.42	2.846	111.7	*x*+1, *y, z*
5	O(7)-H(1W)···N(2)	0.86	2.04	2.823	150.4	-*x*, -*y*+1, -*z*+1
	O(8)-H(3W)···O(10)	0.86	2.36	2.805	112.7	*x*-1, *y*, *z*
	O(8)-H(4W)···N(1)	0.86	2.22	2.755	119.7	-*x*, -*y*, -*z*+2
	O(9)-H(5W)···O(2)	0.85	2.31	2.849	121.5	*x*-1, *y*, *z*
	O(9)-H(6W)···O(4)	0.85	2.23	2.823	127.0	-*x*, -*y*, -*z*+1
	O(10)-H(8W)···N(3)	0.93	1.87	2.775	166	-*x*+1, -*y*+1, -*z*+1
	O(10)-H(7W)···O(3)	0.74	2.14	2.830	153	*x*+1, *y*, *z*
6	O(7)-H(1W)···N(2)	0.87	2.03	2.820	151.3	-*x*+1, -*y*+1, -*z*+1
	O(7)-H(2W)···O(10)	0.87	2.06	2.782	140.7	*x*+1, *y*, *z*
	O(8)-H(3W)···N(1)	0.86	2.08	2.752	135.2	-*x*+1, -*y*, -*z*+2
	O(8)-H(4W)···O(10)	0.86	2.06	2.804	144.7	
	O(9)-H(5W)···O(1)	0.86	2.19	2.861	135.2	*x*-1, *y*, *z*
	O(9)-H(6W)···O(3)	0.86	2.12	2.833	140.2	-*x*+1, -*y*, -*z*+1
	O(10)-H(7W)···O(4)	0.94	2.00	2.810	143	
	O(10)-H(8W)···N(3)	0.74	2.05	2.792	174	-*x*+1, -*y*+1, -*z*+1
7	O(5)-H(1W)···O(8)	0.72	2.52	3.046	131.1	-*x*+1, -*y*, -*z*+1
	O(5)-H(2W)···O(10)	0.87	1.82	2.658	158.7	-*x*+1, -*y*, -*z*+1
	O(6)-H(3W)···N(3)	0.85	2.04	2.803	148.2	*x*, *y*-1, *z*
	O(7)-H(5W)···N(1)	0.85	2.19	2.754	123.1	-*x*+1, -*y*, -*z*+2
	O(7)-H(6W)···O(11)	0.85	2.14	2.748	128.0	*x*-1, *y*-1, *z*
	O(8)-H(7W)···O(2)	0.85	2.55	3.027	116.0	*x*-1, *y*, *z*
	O(8)-H(8W)···O(5)	0.66	2.46	3.046	148.6	-*x*+1, -*y*, -*z*+1
	O(11)-H(9W)···N(2)	0.85	1.99	2.824	166.6	

	O(11)-(10W)···O(10)	0.85	1.91	2.733	162.2	-*x*+1, -*y*+1, -*z*+1
8	O(10)-H(6W)···O(5)	0.74	2.22	2.895	153.2	
	O(10)-H(5W)···N(1)	0.85	1.67	2.530	179.3	-*x*+1, -*y*+1, -*z*+1
	O(9)-H(4W)···O(2)	0.85	1.86	2.711	178.5	*x*+1, *y* , *z*
	O(9)-H(3W)···O(4)	0.85	1.90	2.748	179.2	*x*+1, *y* , *z*
	O(5)-H(1W)···O(1)	0.85	2.13	2.985	179.5	
	O(5)-H(2W)···O(9)	0.87	1.83	2.576	143.4	

Table S3 Summary of thermal analysis data for compounds **1**–**8**.

Compound	T (°C)	Weight loss (%)		Eliminated moieties	T (°C)	Remaining weight (%)		Remaining residue
		exptl	calcd			exptl	calcd	
1	70-160	11.6	11.4	$-4H_2O$	800	28.2	25.8	La_2O_3
2	68-164	11.7	11.4	$-4H_2O$	800	25.7	26.0	Pr_2O_3
3	65-157	11.5	11.3	$-4H_2O$	800	28.1	26.4	Nd_2O_3
4	55-146	11.5	11.2	$-4H_2O$	800	30.1	27.3	Eu_2O_3
5	67-145	10.8	11.1	$-4H_2O$	800	31.0	27.8	Gd_2O_3
6	66-140	10.7	11.0	$-4H_2O$	800	35.0	28.1	Tb_2O_3
7	75-172	13.5	13.2	$-5H_2O$	800	29.5	28.4	Tm_2O_3
8	55-139	5.7	5.9	$-3H_2O$	800	19.6	19.4	Eu_2O_3

Table S4 Luminescent data for compounds **4**, **6**, and **8**.

compound	$\lambda_{max}{}^{a}$ (nm)	assignment	lifetime (ms)	λ excitation/emission (nm)	quantum yield Φ (%)
4	592	$^5D_0 \rightarrow {}^7F_1$			
	615	$^5D_0 \rightarrow {}^7F_2$	0.3	259/616	7.72
	650	$^5D_0 \rightarrow {}^7F_3$			
	698	$^5D_0 \rightarrow {}^7F_4$			
4 dehydrated	590	$^5D_0 \rightarrow {}^7F_1$			
	612	$^5D_0 \rightarrow {}^7F_2$	0.6	259/616	17.17
	651	$^5D_0 \rightarrow {}^7F_3$			
	701	$^5D_0 \rightarrow {}^7F_4$			
4 re-hydrated	592	$^5D_0 \rightarrow {}^7F_1$			
	615	$^5D_0 \rightarrow {}^7F_2$	0.3	259/616	7.58

	649	$^5D_0 \rightarrow {}^7F_3$			
	697	$^5D_0 \rightarrow {}^7F_4$			
6	489	$^5D_4 \rightarrow {}^7F_6$			
	544	$^5D_4 \rightarrow {}^7F_5$	0.8	292/544	12.12
	584	$^5D_4 \rightarrow {}^7F_4$			
	620	$^5D_4 \rightarrow {}^7F_3$			
6 dehydrated	488	$^5D_4 \rightarrow {}^7F_6$			
	544	$^5D_4 \rightarrow {}^7F_5$	1.2	292/543	29.72
	582	$^5D_4 \rightarrow {}^7F_4$			
	622	$^5D_4 \rightarrow {}^7F_3$			
6 re-hydrated	488	$^5D_4 \rightarrow {}^7F_6$			
	543	$^5D_4 \rightarrow {}^7F_5$			
	581	$^5D_4 \rightarrow {}^7F_4$	0.7	292/544	10.86
	620	$^5D_4 \rightarrow {}^7F_3$			
8	591	$^5D_0 \rightarrow {}^7F_1$			
	615	$^5D_0 \rightarrow {}^7F_2$	0.6	330/616	33.65
	653	$^5D_0 \rightarrow {}^7F_3$			
	698	$^5D_0 \rightarrow {}^7F_4$			
8 dehydrated	593	$^5D_0 \rightarrow {}^7F_1$			
	614	$^5D_0 \rightarrow {}^7F_2$	1.1	330/616	86.94
	650	$^5D_0 \rightarrow {}^7F_3$			
	701	$^5D_0 \rightarrow {}^7F_4$			
8 re-hydrated	592	$^5D_0 \rightarrow {}^7F_1$			
	614	$^5D_0 \rightarrow {}^7F_2$	0.5	330/616	31.47
	653	$^5D_0 \rightarrow {}^7F_3$			
	702	$^5D_0 \rightarrow {}^7F_4$			

[a]EX slit = 0.02 nm, and EM slit = 0.02 nm.

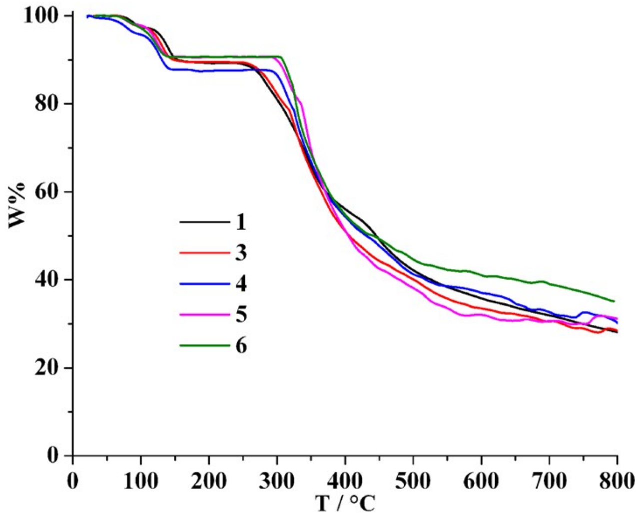
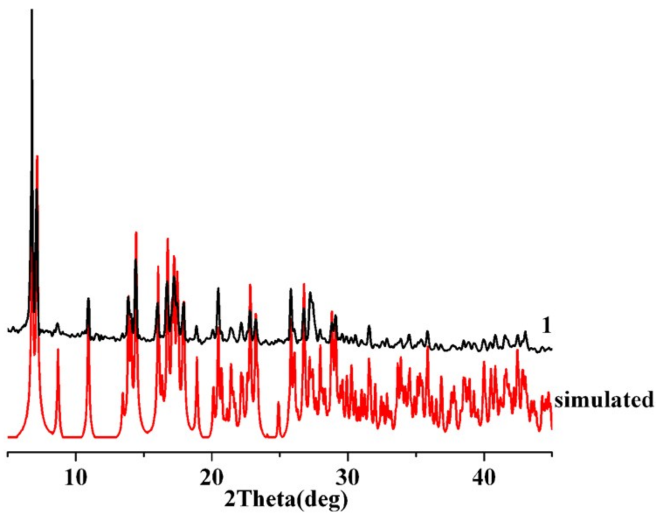
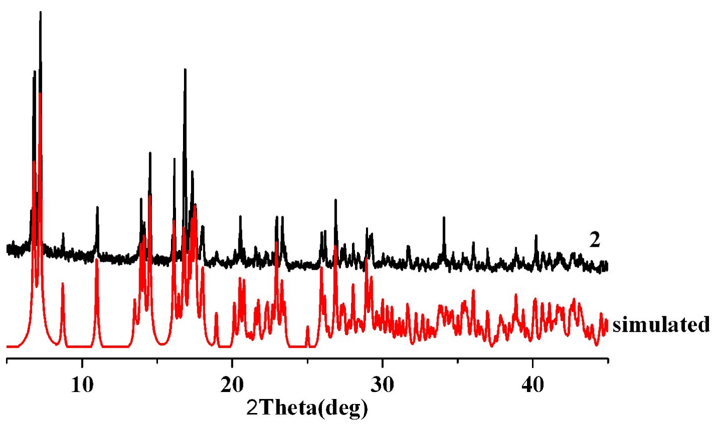
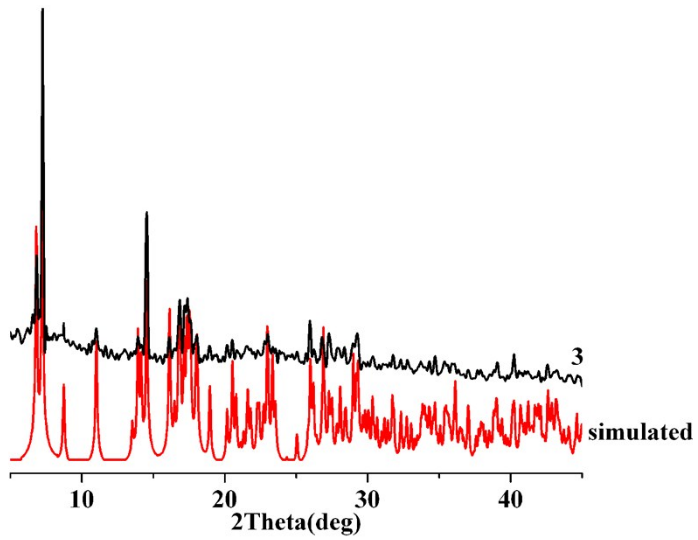
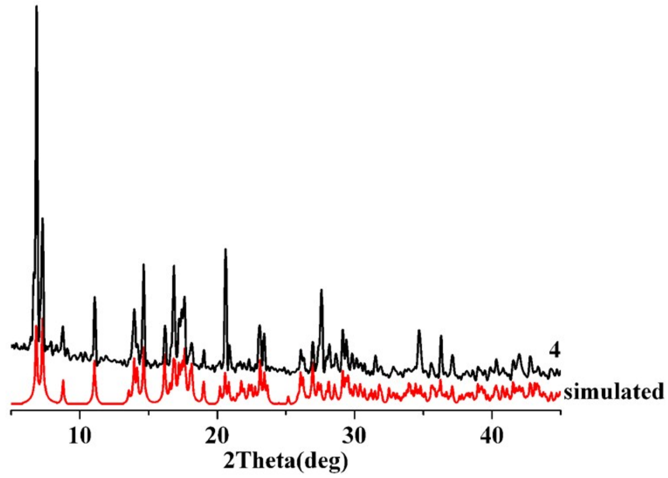


Fig. **S1**. Thermogravimetric analysis (TGA curves) of compounds **1** and **3–6**.






3
simulated
10
20
30
40
2Theta(deg)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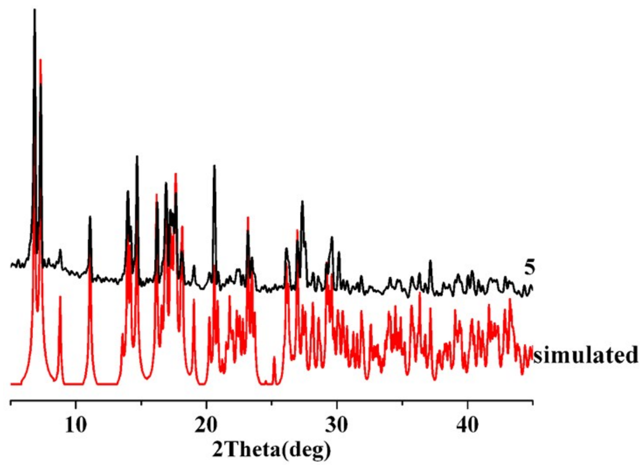
simulated
10
20
30
40
2Theta(deg)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simulated
10
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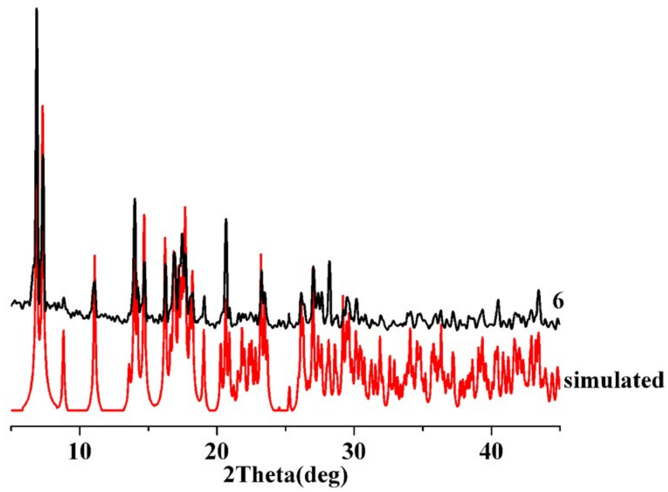
2Theta(deg)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simulated
10
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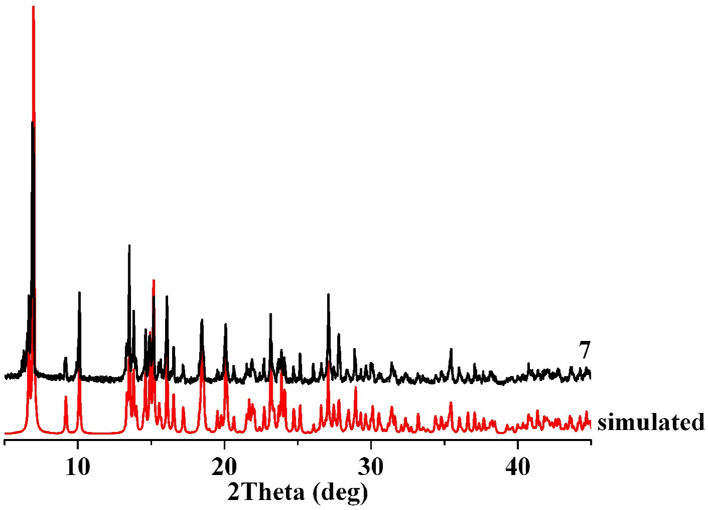
7
simulated
10
20
30
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2Theta (deg)

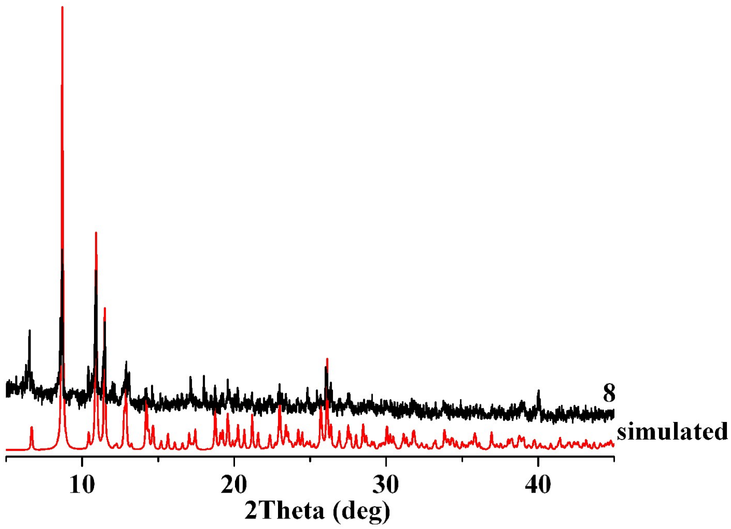

8
simulated
10
20
30
40
2Theta (deg)

Fig. S2 The PXRD patterns of compounds **1**–**8** at room temperature.

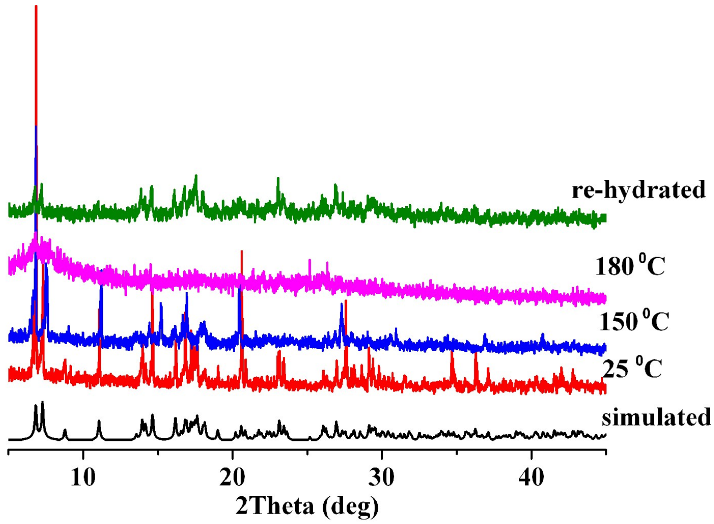


Fig. S3 Results of the temperature-dependent PXRD study of compound **4**.

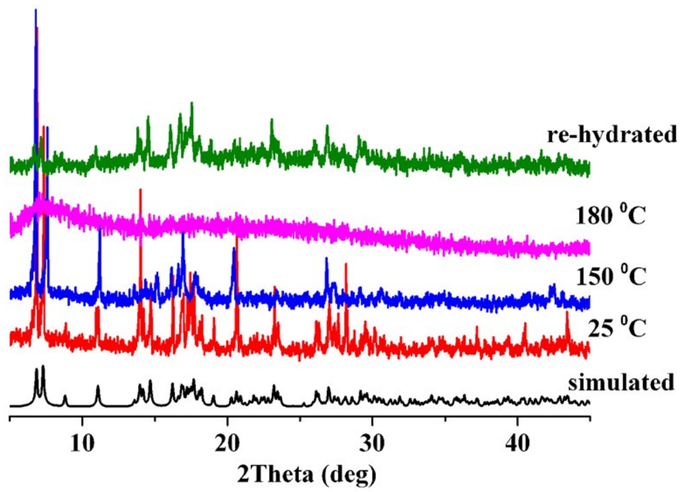


Fig. S4 Results of the temperature-dependent PXRD study of compound **6**.

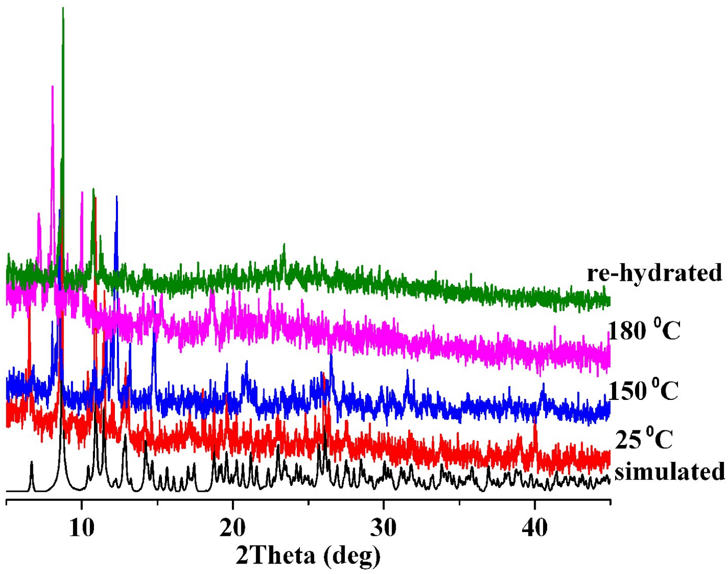
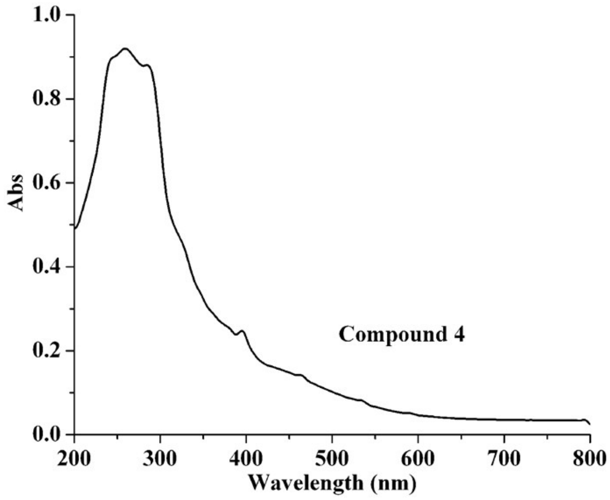
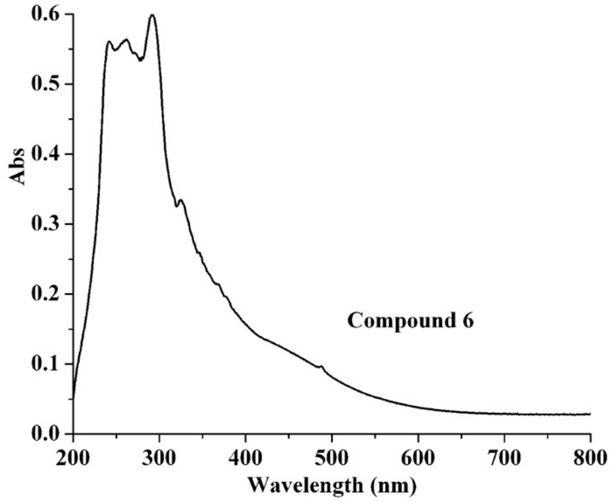


Fig. S5 Results of the temperature-dependent PXRD study of compound **8**.





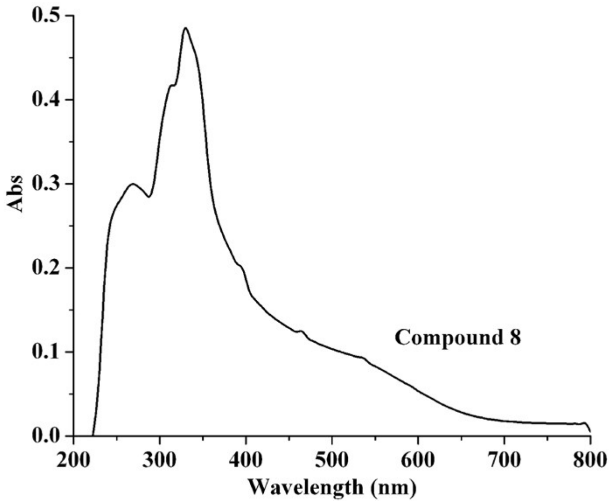


Fig. S6 UV-Vis absorption spectra of compounds **4**, **6** and **8**.

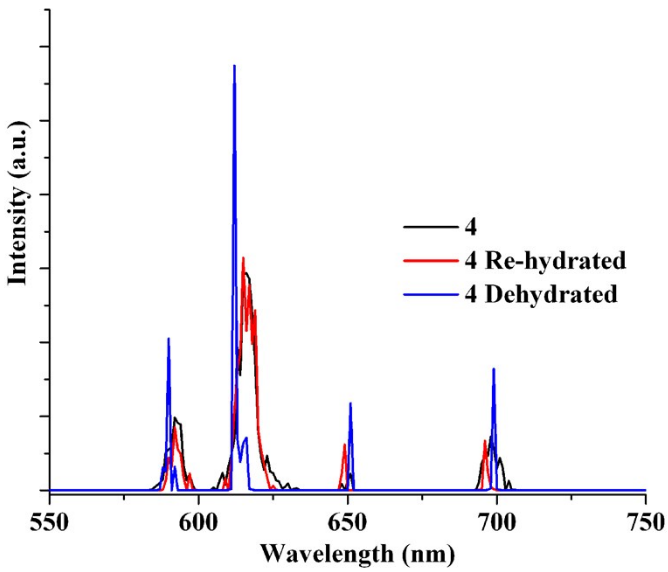


Fig. S7 Solid state emission spectra of compound **4** ($\lambda_{ex.}$ = 259 nm).

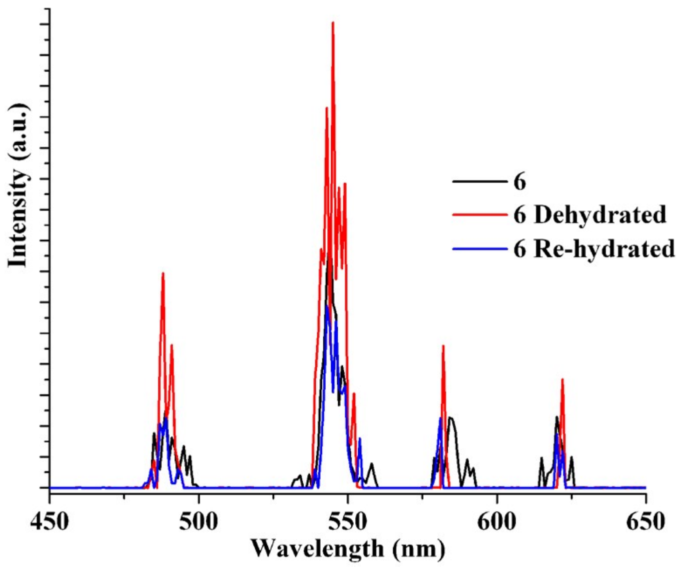


Fig. S8 Solid state emission spectra of compound **6** ($\lambda_{ex.}$ = 292 nm).

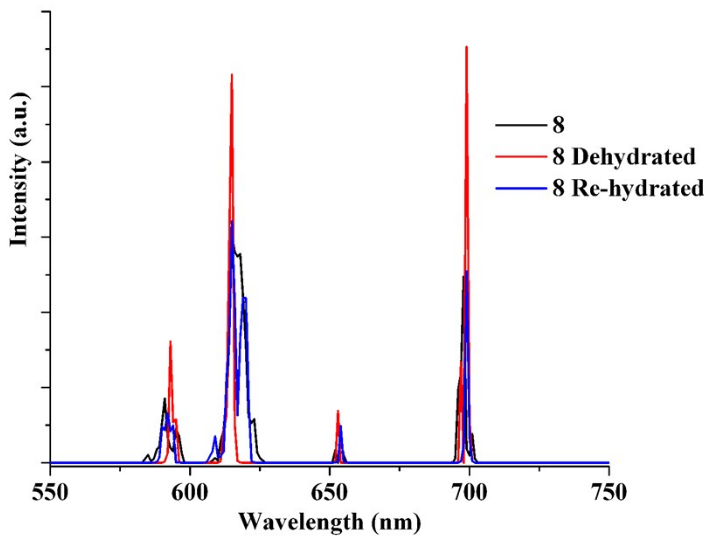


Fig. S9 Solid state emission spectra of compound **8** ($\lambda_{ex.}$ = 330 nm).