Supplementary Material (ESI) for New Journal of Chemistry

Synthesis, crystal structure and luminescence properties of eight new lanthanide carboxyphosphonates with a 3D framework structure

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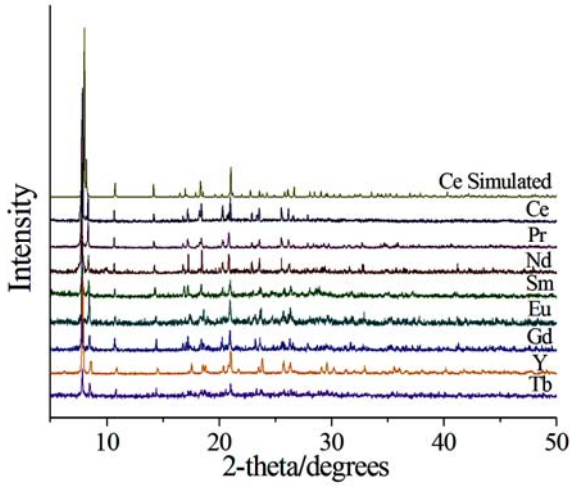

Fig. S1 The simulated XRD pattern of compound **1** (up) and experimental powder XRD patterns of compounds **1–8** (down).

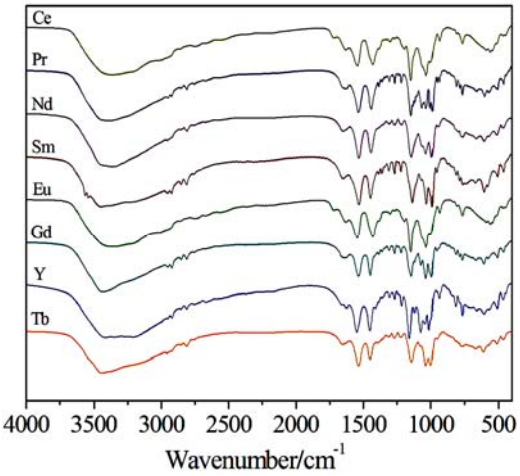

Fig. S2 IR spectra of compounds **1–8**.

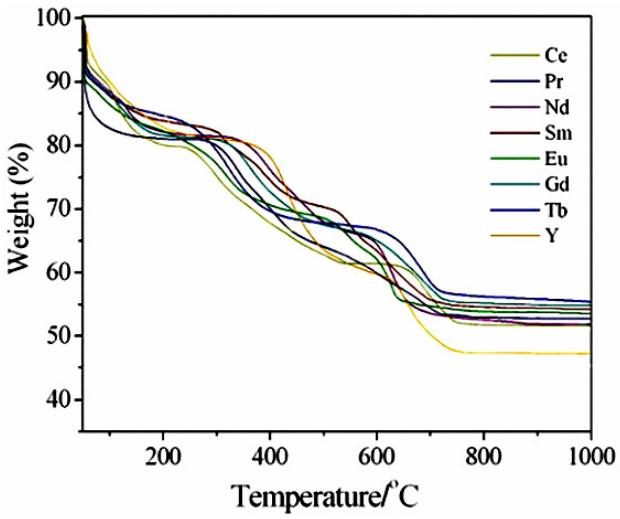

Fig. S3 TGA curves of compounds **1**–**8**.

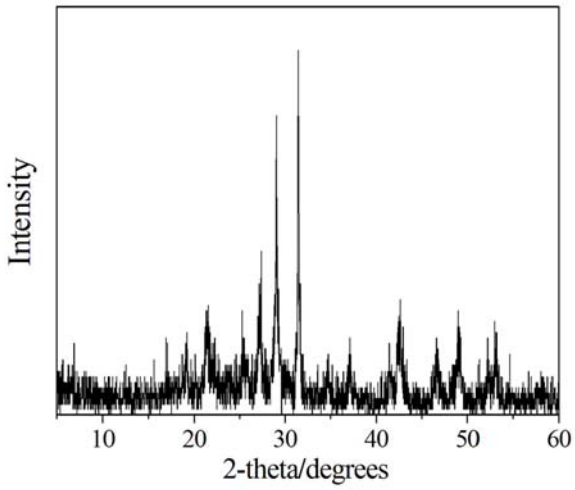

Fig. S4 The X–ray powder diffraction pattern of the final product in the thermal decomposition for compound **3.**

The final product is $NdPO_4$ (JCPDS 00–025–1065).

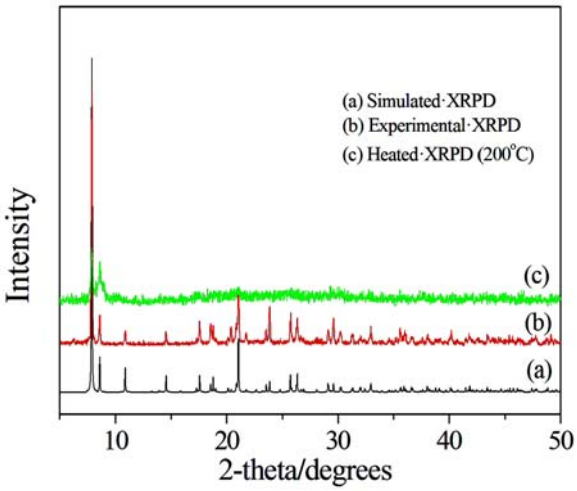

Fig. S5 Experimental and heated (200 °C) X–ray powder diffraction diagram of compound **7** compared to the calculated one.

Table S1. Selected bond lengths (Å) for compounds **1**–**7**

	1 (Ce)	**2** (Pr)	**3** (Nd)	**4** (Sm)	**5** (Eu)	**6** (Gd)	**7** (Y)
Ln(1)–O(1)#1[a]	2.410(7)	2.378(6)	2.357(4)	2.319(10)	2.301(8)	2.284(8)	2.258(5)
Ln(1)–O(3)#2	2.406(8)	2.362(6)	2.343(4)	2.304(11)	2.292(8)	2.296(8)	2.264(5)
Ln(1)–O(7)	2.456(10)	2.457(6)	2.459(5)	2.464(12)	2.419(9)	2.391(8)	2.327(6)
Ln(1)–O(6)	2.484(9)	2.480(6)	2.476(5)	2.441(11)	2.424(9)	2.423(8)	2.362(5)
Ln(1)–O(2)	2.507(8)	2.479(6)	2.469(4)	2.453(10)	2.427(8)	2.422(7)	2.375(5)
Ln(1)–O(4)#3	2.566(8)	2.546(6)	2.545(4)	2.550(11)	2.521(9)	2.506(9)	2.468(6)
Ln(1)–O(1)	2.656(8)	2.607(6)	2.581(4)	2.520(10)	2.524(8)	2.534(8)	2.529(5)
Ln(1)–O(5)#3	2.567(8)	2.548(6)	2.531(5)	2.498(11)	2.485(8)	2.481(8)	2.450(6)

[a] Symmetry transformations used to generate equivalent atoms: #1 –x+1, –y+2, –z+2; #2 –x, –y+2, –z+2; #3 x+1, –y+3/2, z+1/2.

Table S2 Selected angles (°) for compounds **1**–**7**

	1 (Ce)	**2** (Pr)	**3** (Nd)	**4** (Sm)	**5** (Eu)	**6** (Gd)	**7** (Y)
O(1)#1–Ln (1)–O(3)#2[a]	94.3(3)	92.8(2)	93.05(16)	93.3(4)	93.1(3)	93.1(3)	94.5(2)
O(1)#1–Ln (1)–O(7)	161.0(3)	160.6(2)	160.43(16)	160.7(4)	159.9(3)	159.8(3)	158.7(2)
O(3)#2–Ln (1)–O(7)	93.6(3)	92.9(2)	92.55(17)	92.4(4)	92.9(3)	92.7(3)	92.0(2)
O(1)#1–Ln (1)–O(6)	81.3(3)	84.6(2)	85.22(15)	86.0(4)	86.1(3)	85.6(3)	85.04(19)
O(3)#2–Ln (1)–O(6)	160.2(3)	161.9(2)	161.79(16)	162.2(4)	161.2(3)	161.2(3)	160.4(2)
O(7)–Ln (1)–O(6)	96.7(3)	95.5(2)	95.08(17)	94.0(4)	94.2(3)	95.0(3)	95.5(2)
O(1)#1–Ln (1)–O(2)	122.8(2)	124.19(19)	124.80(14)	125.3(3)	125.3(3)	125.6(3)	126.40(18)
O(3)#2–Ln (1)–O(2)	85.2(3)	86.7(2)	86.69(15)	87.2(4)	86.3(3)	86.6(3)	84.65(19)
O(7)–Ln (1)–O(2)	75.1(3)	74.7(2)	74.25(16)	73.4(4)	74.2(3)	74.1(3)	74.4(2)
O(6)–Ln (1)–O(2)	81.2(3)	80.0(2)	79.54(15)	78.8(4)	78.9(3)	79.0(3)	79.97(19)
O(1)#1–Ln (1)–O(4)#3	80.4(3)	82.5(2)	82.61(16)	83.1(4)	82.8(3)	82.7(3)	82.3(2)
O(3)#2–Ln (1)–O(4)#3	124.4(3)	124.4(2)	124.66(15)	125.3(4)	125.9(3)	126.2(3)	126.62(19)
O(7)–Ln (1)–O(4)#3	80.8(3)	78.9(2)	78.78(17)	78.6(4)	78.1(3)	78.3(3)	77.6(2)
O(6)–Ln (1)–O(4)#3	74.1(3)	73.2(2)	73.16(15)	72.4(4)	72.7(3)	72.3(3)	72.83(19)
O(2)–Ln (1)–O(4)#3	143.0(3)	140.1(2)	139.38(15)	137.8(4)	138.4(3)	137.8(3)	138.46(19)
O(1)#1–Ln (1)–O(1)	66.6(3)	67.3(2)	67.28(15)	67.3(4)	67.1(3)	67.0(3)	67.12(19)
O(3)#2–Ln (1)–O(1)	84.5(3)	85.3(2)	85.22(15)	84.6(4)	84.7(3)	84.5(3)	84.76(18)
O(7)–Ln (1)–O(1)	131.5(3)	131.7(2)	131.93(15)	131.7(3)	132.6(3)	132.9(3)	133.80(19)
O(6)–Ln (1)–O(1)	76.0(3)	77.2(2)	77.38(15)	78.7(4)	77.7(3)	77.6(3)	76.94(18)
O(2)–Ln (1)–O(1)	56.4(2)	57.02(18)	57.68(13)	58.3(3)	58.4(3)	58.8(3)	59.42(16)
O(4)#3–Ln (1)–O(1)	138.2(3)	139.3(2)	139.24(15)	139.7(4)	138.8(3)	138.6(3)	138.39(18)
O(1)#1–Ln (1)–O(5)#3	82.6(3)	82.9(2)	83.45(16)	84.9(4)	84.1(3)	84.1(3)	82.3(2)
O(3)#2–Ln (1)–O(5)#3	74.3(3)	73.9(2)	73.90(15)	74.0(4)	74.1(3)	74.1(3)	74.16(19)
O(7)–Ln (1)–O(5)#3	82.9(3)	80.9(2)	80.12(18)	79.0(4)	79.2(3)	78.9(3)	80.0(2)
O(6)–Ln (1)–O(5)#3	123.7(3)	123.4(2)	123.72(16)	123.6(4)	124.4(3)	124.3(3)	125.01(19)
O(2)–Ln (1)–O(5)#3	148.9(3)	147.9(2)	147.00(17)	145.8(4)	145.9(3)	145.8(3)	146.0(2)
O(4)#3–Ln (1)–O(5)#3	50.1(3)	50.5(2)	50.76(15)	51.3(4)	51.8(3)	52.2(3)	52.54(18)
O(1)–Ln (1)–O(5)#3	141.0(3)	142.7(2)	143.04(15)	143.8(4)	143.1(3)	143.0(3)	141.28(19)

[a] Symmetry transformations used to generate equivalent atoms: #1 –x+1, –y+2, –z+2; #2 –x, –y+2, –z+2; #3 x+1, –y+3/2, z+1/2.