Supplementary Material (ESI) for New Journal of Chemistry

Synthesis, crystal structure and luminescence property of lanthanide oxalatophosphonates with a three-dimensional framework structure

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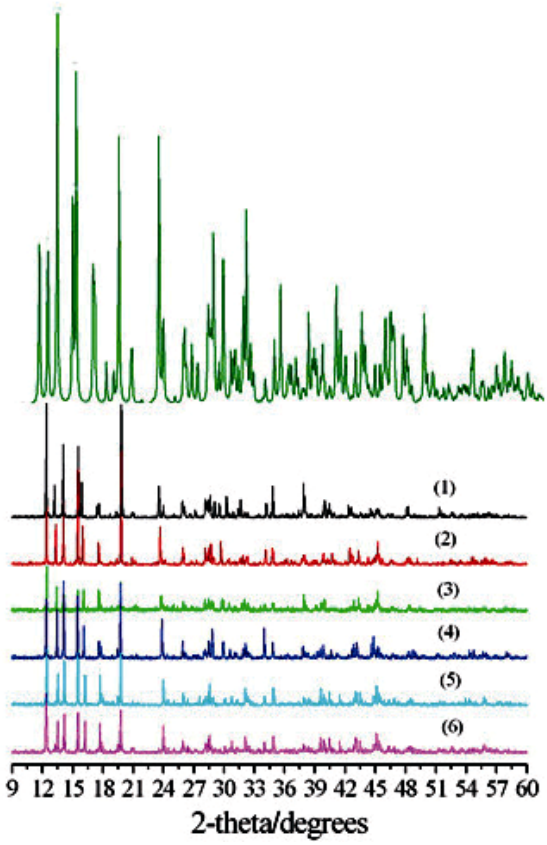

Fig. S1 The simulated XRD pattern of compound **1** (up) and the experimental powder XRD patterns of compounds **1–6** (down).

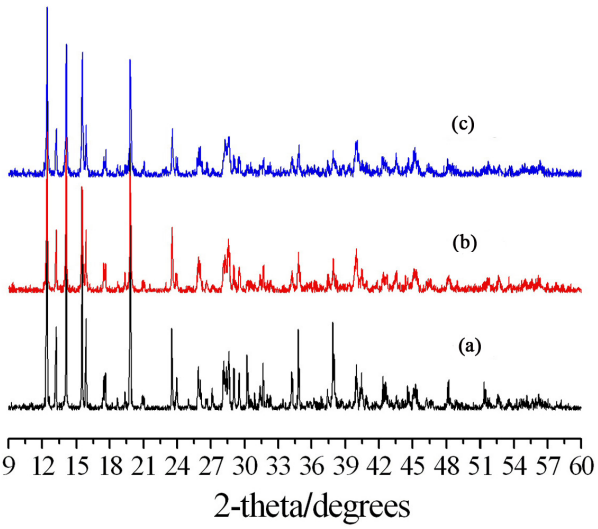

Fig. S2 The experimental powder XRD pattern of compound **1** (*a*), dehydrated sample after calcination at 150 °C (b), 180 °C (c).

Table S1 Selected bond lengths (Å) for compounds **1**–**6**

	1 (La)	**2** (Ce)	**3** (Pr)	**4** (Nd)	**5** (Sm)	**6** (Eu)
Ln(1)–O(3)#1[a]	2.415(2)	2.389(3)	2.372(3)	2.360(3)	2.336(3)	2.330(3)
Ln(1)–O(2)	2.515(2)	2.492(3)	2.481(3)	2.471(3)	2.449(4)	2.439(3)
Ln(1)–O(7)	2.535(3)	2.510(3)	2.493(3)	2.476(3)	2.454(4)	2.449(3)
Ln(1)–O(6)#2	2.557(2)	2.538(3)	2.522(3)	2.504(3)	2.485(3)	2.480(3)
Ln(1)–O(5)	2.587(2)	2.574(3)	2.559(3)	2.545(3)	2.521(3)	2.518(3)
Ln(1)–O(9)	2.594(3)	2.562(3)	2.537(4)	2.520(4)	2.484(5)	2.476(3)
Ln(1)–O(8)#3	2.599(2)	2.580(3)	2.571(3)	2.557(3)	2.542(4)	2.537(3)
Ln(1)–O(10)	2.609(3)	2.571(3)	2.542(4)	2.523(4)	2.485(4)	2.472(3)
Ln(1)–O(4)#2	2.610(2)	2.595(3)	2.573(3)	2.563(3)	2.544(3)	2.542(3)

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

Table S2 Selected angles (°) for compounds **1–6**

	1 (La)	**2** (Ce)	**3** (Pr)	**4** (Nd)	**5** (Sm)	**6** (Eu)
O(2)–Ln(1)–O(3)#1[a]	74.39(8)	74.69(9)	74.73(11)	74.73(11)	74.78(12)	74.73(10)
O(7)–Ln(1)–O(3)#1	134.77(8)	134.80(9)	134.96(11)	135.08(11)	135.31(12)	135.34(10)
O(2)–Ln(1)–O(7)	140.07(8)	139.07(9)	138.41(11)	138.14(11)	137.81(12)	137.73(10)
O(3)#1–Ln(1)–O(6)#2	83.68(8)	84.57(9)	84.84(11)	85.16(10)	85.22(12)	85.33(9)
O(2)–Ln(1)–O(6)#2	75.69(7)	75.10(9)	74.61(10)	74.08(10)	73.51(12)	73.34(9)
O(7)–Ln(1)–O(6)#2	125.53(8)	126.09(9)	126.65(11)	126.87(10)	127.17(12)	127.28(9)
O(3)#1–Ln(1)–O(5)	95.40(9)	95.35(10)	95.17(12)	94.99(11)	94.97(13)	94.87(10)
O(2)–Ln(1)–O(5)	71.43(7)	71.48(8)	71.74(11)	71.91(10)	72.08(12)	72.15(9)
O(7)–Ln(1)–O(5)	78.11(8)	77.15(9)	76.40(11)	76.14(10)	75.85(12)	75.73(10)
O(6)#2–Ln(1)–O(5)	146.03(8)	145.28(9)	145.04(12)	144.63(11)	144.22(13)	144.10(10)
O(3)#1–Ln(1)–O(9)	142.17(9)	142.47(10)	142.45(12)	142.41(12)	142.52(14)	142.57(11)
O(2)–Ln(1)–O(9)	68.21(8)	67.98(10)	67.83(11)	67.73(11)	67.77(13)	67.85(10)
O(7)–Ln(1)–O(9)	80.96(9)	79.89(10)	79.20(12)	78.74(12)	78.11(13)	77.83(10)
O(6)#2–Ln(1)–O(9)	81.90(9)	82.32(10)	82.73(13)	82.89(12)	83.11(14)	83.32(11)
O(5)–Ln(1)–O(9)	78.27(9)	76.79(10)	76.14(12)	75.58(12)	75.13(14)	74.87(11)
O(3)#1–Ln(1)–O(8)#3	72.58(8)	71.85(9)	71.61(10)	71.28(10)	70.88(12)	70.85(9)
O(2)–Ln(1)–O(8)#3	126.02(8)	126.40(9)	126.70(11)	126.87(10)	126.91(12)	127.13(10)
O(7)–Ln(1)–O(8)#3	62.98(8)	63.46(9)	63.71(10)	64.08(10)	64.66(11)	64.68(9)
O(6)#2–Ln(1)–O(8)#3	139.23(8)	139.41(10)	139.46(11)	139.60(11)	139.63(13)	139.56(10)
O(5)–Ln(1)–O(8)#3	70.60(8)	71.36(10)	71.53(12)	71.76(12)	71.98(13)	72.18(11)
O(9)–Ln(1)–O(8)#3	135.96(9)	135.49(10)	135.15(12)	135.00(12)	134.93(14)	134.76(11)
O(3)#1–Ln(1)–O(10)	75.04(9)	75.68(10)	76.10(12)	76.26(12)	76.58(14)	76.72(11)
O(2)–Ln(1)–O(10)	138.18(9)	138.37(11)	138.25(12)	137.96(12)	137.90(14)	137.88(12)
O(7)–Ln(1)–O(10)	81.51(9)	82.24(11)	82.97(13)	83.46(13)	83.76(14)	83.85(12)
O(6)#2–Ln(1)–O(10)	73.19(9)	73.59(11)	73.61(13)	73.76(13)	73.95(15)	74.08(12)
O(5)–Ln(1)–O(10)	139.47(9)	140.09(11)	140.38(13)	140.66(13)	140.93(15)	140.93(12)
O(9)–Ln(1)–O(10)	132.27(9)	132.49(10)	132.61(13)	132.88(12)	132.78(14)	132.87(11)
O(8)#3–Ln(1)–O(10)	68.96(10)	68.89(11)	69.03(14)	69.09(13)	69.21(15)	69.01(12)
O(3)#1–Ln(1)–O(4)#2	134.41(8)	135.64(9)	136.25(11)	136.76(10)	137.15(13)	137.31(9)
O(2)–Ln(1)–O(4)#2	117.96(7)	117.50(9)	117.27(10)	117.02(10)	116.85(12)	116.89(9)
O(7)–Ln(1)–O(4)#2	65.21(7)	65.21(8)	65.32(10)	65.23(10)	65.04(12)	64.99(9)
O(6)#2–Ln(1)–O(4)#2	60.76(7)	61.20(8)	61.58(10)	61.83(9)	62.29(11)	62.43(9)
O(5)–Ln(1)–O(4)#2	130.11(8)	128.93(9)	128.51(11)	128.18(10)	127.80(12)	127.73(9)
O(9)–Ln(1)–O(4)#2	64.06(8)	64.08(9)	64.28(11)	64.40(11)	64.39(13)	64.54(10)
O(8)#3–Ln(1)–O(4)#2	115.73(7)	115.78(9)	115.71(10)	115.80(10)	115.94(12)	115.70(10)
O(10)–Ln(1)–O(4)#2	68.27(9)	68.44(10)	68.36(12)	68.51(11)	68.41(13)	68.35(11)

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