Supplementary Material (ESI) for Dalton Transactions


# Hydrothermal synthesis, crystal structures, and luminescent properties of a series of new lanthanide oxalatophosphonates with a layer architecture

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## Supporting Information

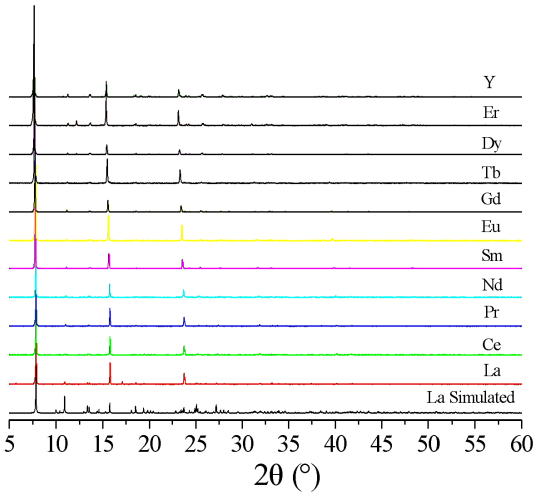


**Fig. S1** The X-ray powder diffraction patterns of the samples of **1–11** and the simulated XRD pattern of compound **1**.

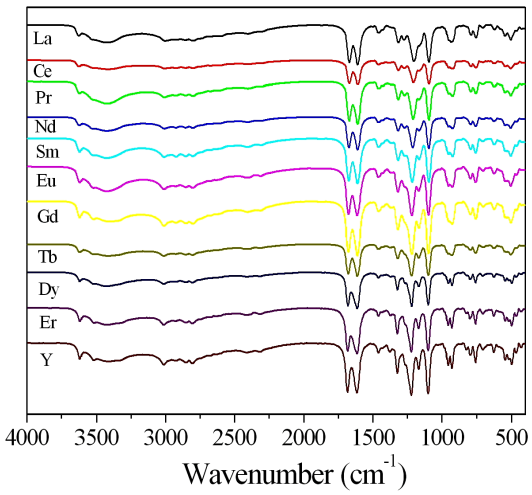


**Fig. S2** The IR spectra of compounds **1–11.**

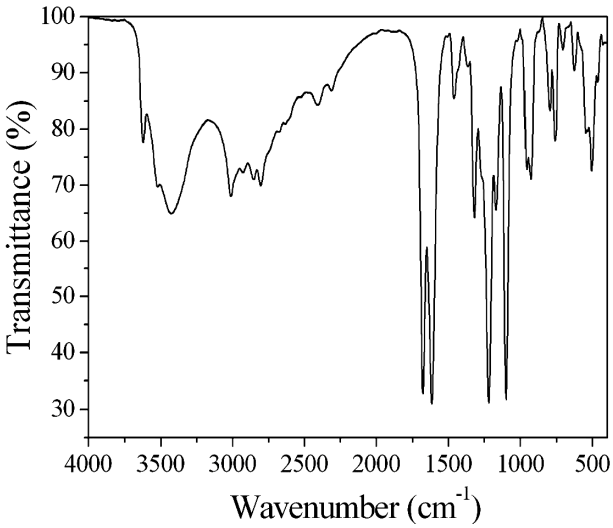


**Fig. S3** The IR spectrum of compound **6.**

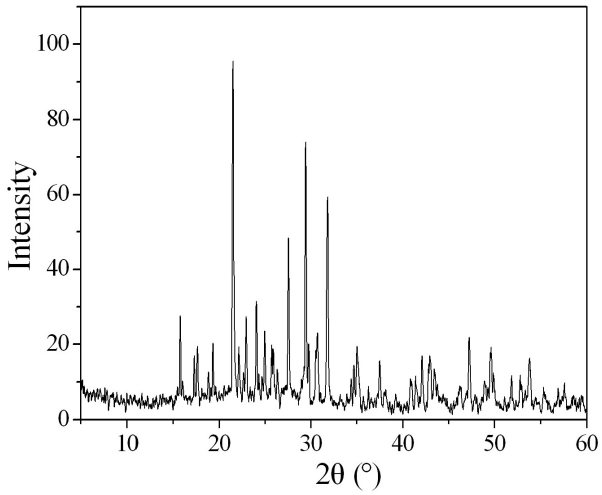


**Fig. S4** The X-ray powder diffraction pattern of the final product in the thermal decomposition for compound **6.** The final product is mixture of $Eu(PO_3)_3$ and $EuPO_4$ (JCPDS 00–034–1453 and 01–083–0656).

**Table S1** Selected Bond Lengths (Å) for Compounds **1**–**7**

| | **1** (La) | **2** (Ce) | **3** (Pr) | **4** (Nd) | **5** (Sm) | **6** (Eu) | **7** (Gd) |
|---|---|---|---|---|---|---|---|
| Ln(1)–O(2)#1[a] | 2.410(4) | 2.391(2) | 2.372(4) | 2.361(4) | 2.333(5) | 2.324(3) | 2.324(5) |
| Ln(1)–O(1) | 2.445(4) | 2.416(2) | 2.390(4) | 2.375(4) | 2.346(5) | 2.336(3) | 2.330(5) |
| Ln(1)–O(4) | 2.478(4) | 2.456(2) | 2.437(4) | 2.423(4) | 2.392(4) | 2.380(3) | 2.384(5) |
| Ln(1)–O(8)#2 | 2.517(4) | 2.491(2) | 2.474(4) | 2.466(4) | 2.433(5) | 2.426(3) | 2.429(5) |
| Ln(1)–O(7) | 2.547(4) | 2.527(2) | 2.510(4) | 2.496(4) | 2.480(5) | 2.463(3) | 2.457(5) |
| Ln(1)–O(5)#1 | 2.559(4) | 2.538(2) | 2.515(4) | 2.498(4) | 2.456(5) | 2.451(3) | 2.438(5) |
| Ln(1)–O(10)#2 | 2.581(4) | 2.557(2) | 2.536(4) | 2.510(4) | 2.485(5) | 2.469(3) | 2.465(5) |
| Ln(1)–O(9) | 2.591(4) | 2.568(2) | 2.549(4) | 2.523(5) | 2.494(5) | 2.478(3) | 2.465(5) |
| P(1)–O(1) | 1.494(4) | 1.496(2) | 1.498(4) | 1.499(5) | 1.493(5) | 1.492(3) | 1.496(5) |
| P(1)–O(2) | 1.498(4) | 1.498(2) | 1.491(4) | 1.493(4) | 1.495(5) | 1.498(3) | 1.498(5) |
| P(1)–O(3) | 1.556(4) | 1.558(2) | 1.555(4) | 1.554(5) | 1.550(5) | 1.555(3) | 1.551(6) |
| P(1)–C(1) | 1.829(6) | 1.821(3) | 1.817(6) | 1.810(6) | 1.812(7) | 1.821(5) | 1.820(8) |
| P(2)–O(4) | 1.492(4) | 1.488(2) | 1.482(4) | 1.484(4) | 1.480(5) | 1.481(3) | 1.474(5) |
| P(2)–O(5) | 1.515(4) | 1.512(2) | 1.506(4) | 1.503(5) | 1.509(5) | 1.511(3) | 1.504(5) |
| P(2)–O(6) | 1.563(4) | 1.569(2) | 1.572(4) | 1.572(4) | 1.568(5) | 1.569(3) | 1.575(5) |
| P(2)–C(2) | 1.823(6) | 1.832(4) | 1.831(6) | 1.829(7) | 1.817(8) | 1.825(5) | 1.841(8) |

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

**Table S2** Selected Bond Angles (°) for Compounds **1**–**7**

| | **1** (La) | **2** (Ce) | **3** (Pr) | **4** (Nd) | **5** (Sm) | **6** (Eu) | **7** (Gd) |
|---|---|---|---|---|---|---|---|
| O(2)#1[a]–Ln(1)–O(1) | 127.44(13) | 126.34(7) | 124.95(12) | 124.33(16) | 123.13(18) | 122.63(10) | 122.48(18) |
| O(2)#1–Ln(1)–O(4) | 78.15(13) | 78.03(8) | 77.81(12) | 77.58(15) | 77.72(16) | 77.75(11) | 77.74(17) |
| O(1)–Ln(1)–O(4) | 74.53(13) | 74.91(8) | 75.16(12) | 75.49(15) | 75.87(16) | 75.82(11) | 75.73(17) |
| O(2)#1–Ln(1)–O(8)#2 | 84.73(12) | 84.50(7) | 84.79(12) | 84.46(15) | 84.18(17) | 83.75(11) | 83.43(18) |
| O(1)–Ln(1)–O(8)#2 | 137.03(12) | 137.46(8) | 137.74(13) | 138.02(15) | 138.17(16) | 138.29(10) | 138.59(17) |
| O(4)–Ln(1)–O(8)#2 | 146.89(13) | 146.36(8) | 146.01(13) | 145.62(16) | 145.32(18) | 145.45(11) | 145.30(18) |
| O(2)#1–Lna(1)–O(7) | 135.15(12) | 135.72(8) | 136.39(13) | 136.89(14) | 137.60(16) | 137.84(10) | 137.78(18) |
| O(1)–Ln(1)–O(7) | 75.34(12) | 75.83(7) | 76.41(12) | 76.35(15) | 77.26(17) | 77.55(10) | 77.75(17) |
| O(4)–Ln(1)–O(7) | 71.98(13) | 71.86(8) | 71.94(13) | 71.95(15) | 72.03(17) | 72.11(10) | 72.13(18) |
| O(8)#2–Ln(1)–O(7) | 102.70(13) | 103.28(8) | 103.41(12) | 104.21(15) | 104.53(17) | 105.16(10) | 105.36(18) |
| O(2)#1–Ln(1)–O(5)#1 | 73.50(12) | 73.46(8) | 73.55(13) | 73.49(15) | 73.10(16) | 73.55(11) | 73.83(18) |
| O(1)–Ln(1)–O(5)#1 | 86.19(13) | 84.84(8) | 83.18(13) | 82.45(16) | 81.25(17) | 80.11(11) | 79.41(18) |
| O(4)–Ln(1)–O(5)#1 | 124.26(12) | 124.08(7) | 123.71(12) | 123.52(16) | 123.50(17) | 123.20(10) | 122.78(18) |
| O(8)#2–Ln(1)–O(5)#1 | 76.11(13) | 76.55(8) | 77.41(12) | 77.49(15) | 77.55(17) | 77.66(10) | 78.15(18) |
| O(7)–Ln(1)–O(5)#1 | 151.35(12) | 150.82(8) | 149.99(13) | 149.48(15) | 149.13(17) | 148.37(10) | 148.10(17) |
| O(2)#1–Ln(1)–O(10)#2 | 141.74(13) | 141.70(8) | 142.32(13) | 142.47(15) | 142.28(16) | 142.54(11) | 142.72(18) |
| O(1)–Ln(1)–O(10)#2 | 74.96(12) | 75.23(7) | 75.36(12) | 75.17(15) | 75.52(17) | 75.64(10) | 75.72(17) |
| O(4)–Ln(1)–O(10)#2 | 139.98(13) | 140.12(8) | 139.71(13) | 139.74(15) | 139.77(16) | 139.48(11) | 139.32(17) |
| O(8)#2–Ln(1)–O(10)#2 | 63.37(12) | 63.81(7) | 64.29(12) | 65.01(15) | 65.29(17) | 65.74(11) | 66.14(18) |
| O(7)–Ln(1)–O(10)#2 | 75.71(13) | 75.66(8) | 74.89(14) | 74.78(15) | 74.52(18) | 74.10(11) | 73.95(19) |
| O(5)#1–Ln(1)–O(10)#2 | 78.47(13) | 78.42(8) | 78.83(13) | 78.76(15) | 78.85(17) | 78.88(10) | 79.05(18) |
| O(2)#1–Ln(1)–O(9) | 79.20(13) | 79.38(8) | 79.74(13) | 79.81(15) | 80.32(17) | 79.93(11) | 79.81(18) |
| O(1)–Ln(1)–O(9) | 136.52(12) | 137.33(8) | 138.32(13) | 138.76(15) | 139.44(16) | 140.21(11) | 140.53(18) |
| O(4)–Ln(1)–O(9) | 79.99(13) | 79.47(8) | 79.33(13) | 78.96(16) | 78.40(17) | 78.49(11) | 78.73(19) |
| O(8)#2–Ln(1)–O(9) | 69.01(14) | 69.12(8) | 68.90(13) | 69.09(16) | 69.49(17) | 69.63(11) | 69.36(19) |
| O(7)–Ln(1)–O(9) | 63.43(12) | 63.94(7) | 64.52(12) | 65.15(15) | 65.18(17) | 65.85(10) | 65.97(17) |
| O(5)#1–Ln(1)–O(9) | 137.18(13) | 137.77(8) | 138.47(13) | 138.78(15) | 139.31(17) | 139.68(11) | 140.05(18) |
| O(10)#2–Ln(1)–O(9) | 105.91(14) | 106.28(8) | 106.21(13) | 106.76(16) | 106.91(18) | 107.10(11) | 106.97(19) |

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