

ELECTRONIC SUPPLEMENTARY INFORMATION

Self-Assembly of lanthanide (III) coordination polymers from a bifunctional 2-(pyridin-2-yl)-1H-imidazole-4,5-dicarboxylate ligand with the assistance of oxalate: syntheses, structures, luminescence, and magnetic properties

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Table S1. Selected bond lengths(Å) and bond angles(°) of compounds 1-11.

Table S2. Hydrogen bonds for compounds 1-11.

Table S3. Synthesis procedures.

Table S4. Elemental analysis and IR results of complexes 1-11.

Figure S1. TGA curves for complexes 1 and 3.

Figure S2. The total solid-state luminescent spectra of complexes 1-11.

Figure S3 Plots of χ_M (left), $\chi_M T$ (right) and χ_M^{-1} (insert) vs T for Ln(III) in 8-11.

Table S1. Selected bond lengths (Å) and bond angles (°)

1					
La1–O3 ⁱ	2.435 (3)	La1–O4	2.521 (3)	La1–O5 ⁱⁱⁱ	2.588 (3)
La1–O1 ⁱⁱ	2.476 (3)	La1–O6	2.567 (2)	La1–O7	2.659 (3)
La1–O2 ⁱ	2.480 (3)	La1–N2	2.572 (3)		
O3 ⁱ –La1–O1 ⁱⁱ	71.03 (10)	O3 ⁱ –La1–N2	149.35 (9)	O6–La1–O5 ⁱⁱⁱ	63.19 (8)
O3 ⁱ –La1–O2 ⁱ	73.15 (9)	O1 ⁱⁱ –La1–N2	127.59 (10)	N2–La1–O5 ⁱⁱⁱ	70.89 (9)
O1 ⁱⁱ –La1–O2 ⁱ	122.45 (10)	O2 ⁱ –La1–N2	76.20 (9)	O3 ⁱ –La1–O7	66.86 (12)
O3 ⁱ –La1–O4	107.80 (11)	O4–La1–N2	61.27 (9)	O1 ⁱⁱ –La1–O7	130.37 (11)
O1 ⁱⁱ –La1–O4	77.87 (9)	O6–La1–N2	118.87 (9)	O2 ⁱ –La1–O7	67.96 (11)
O2 ⁱ –La1–O4	72.13 (11)	O3 ⁱ –La1–O5 ⁱⁱⁱ	138.86 (9)	O4–La1–O7	139.51 (11)
O3 ⁱ –La1–O6	88.19 (9)	O1 ⁱⁱ –La1–O5 ⁱⁱⁱ	72.76 (9)	O6–La1–O7	79.86 (10)
O1 ⁱⁱ –La1–O6	73.67 (8)	O2 ⁱ –La1–O5 ⁱⁱⁱ	145.37 (9)	N2–La1–O7	101.89 (11)
O2 ⁱ –La1–O6	147.04 (10)	O4–La1–O5 ⁱⁱⁱ	82.70 (9)	O5 ⁱⁱⁱ –La1–O7	129.05 (9)
O4–La1–O6	140.55 (9)				

Symmetry codes: (i) $x-1/2, -y+1/2, z+1/2$; (ii) $x, y, z+1$; (iii) $-x+1, -y, -z+2$; (iv) $x, y, z-1$; (v) $x+1/2, -y+1/2, z-1/2$.

2

Ce1–O3 ⁱ	2.415 (2)	Ce1–O4	2.510 (2)	Ce1–O5 ⁱⁱⁱ	2.573 (2)
Ce1–O2 ⁱ	2.462 (2)	Ce1–O6	2.542 (2)	Ce1–O7	2.625 (3)
Ce1–O1 ⁱⁱ	2.468 (2)	Ce1–N2	2.545 (3)		
O3 ⁱ –Ce1–O2 ⁱ	74.26 (7)	O3 ⁱ –Ce1–N2	150.05 (8)	O6–Ce1–O5 ⁱⁱⁱ	63.87 (7)
O3 ⁱ –Ce1–O1 ⁱⁱ	70.96 (8)	O2 ⁱ –Ce1–N2	75.80 (8)	N2–Ce1–O5 ⁱⁱⁱ	70.78 (8)
O2 ⁱ –Ce1–O1 ⁱⁱ	122.73 (8)	O1 ⁱⁱ –Ce1–N2	126.83 (8)	O3 ⁱ –Ce1–O7	67.43 (10)

O3 ⁱ –Ce1–O4	107.24 (8)	O4–Ce1–N2	61.89 (8)	O2 ⁱ –Ce1–O7	67.94 (9)
O2 ⁱ –Ce1–O4	71.94 (8)	O6–Ce1–N2	119.32 (7)	O1 ⁱⁱ –Ce1–O7	131.27 (9)
O1 ⁱⁱ –Ce1–O4	76.79 (7)	O3 ⁱ –Ce1–O5 ⁱⁱⁱ	138.10 (7)	O4–Ce1–O7	139.43 (9)
O3 ⁱ –Ce1–O6	87.30 (7)	O2 ⁱ –Ce1–O5 ⁱⁱⁱ	144.71 (7)	O6–Ce1–O7	80.05 (8)
O2 ⁱ –Ce1–O6	147.19 (8)	O1 ⁱⁱ –Ce1–O5 ⁱⁱⁱ	72.03 (7)	N2–Ce1–O7	101.77 (9)
O1 ⁱⁱ –Ce1–O6	73.71 (7)	O4–Ce1–O5 ⁱⁱⁱ	82.45 (8)	O5 ⁱⁱⁱ –Ce1–O7	129.66 (8)
O4–Ce1–O6	140.50 (7)				

Symmetry codes: (i) $x-1/2, -y+1/2, z+1/2$; (ii) $x, y, z+1$; (iii) $-x+1, -y, -z+2$; (iv) $x, y, z-1$; (v) $x+1/2, -y+1/2, z-1/2$.

3

Pr1–O12 ⁱ	2.390 (2)	Pr1–O2	2.527 (2)	Pr2–O15	2.505 (2)
Pr1–O10 ⁱ	2.419 (2)	Pr1–O6	2.567 (2)	Pr2–N1	2.506 (3)
Pr1–O13 ⁱⁱ	2.456 (2)	Pr2–O3	2.472 (2)	Pr2–O11	2.540 (2)
Pr1–O1	2.472 (2)	Pr2–O8	2.491 (2)	Pr2–O4	2.545 (2)
Pr1–O7	2.484 (2)	Pr2–O9 ⁱⁱⁱ	2.498 (2)	Pr2–N3	2.846 (3)
Pr1–O5	2.510 (2)	Pr2–O14 ^{iv}	2.500 (2)	O10 ⁱ –Pr1–O6	73.47 (7)
O12 ⁱ –Pr1–O10 ⁱ	77.80 (7)	O10 ⁱ –Pr1–O5	144.55 (7)	O13 ⁱⁱ –Pr1–O6	73.22 (8)
O12 ⁱ –Pr1–O13 ⁱⁱⁱ	146.16 (8)	O13 ⁱⁱ –Pr1–O5	75.64 (8)	O1–Pr1–O6	139.72 (8)
O10 ⁱ –Pr1–O13 ⁱⁱⁱ	81.86 (8)	O1–Pr1–O5	75.55 (7)	O7–Pr1–O6	143.99 (7)
O12 ⁱ –Pr1–O1	139.63 (8)	O7–Pr1–O5	141.29 (7)	O5–Pr1–O6	73.99 (7)
O10 ⁱ –Pr1–O1	123.99 (7)	O12 ⁱ –Pr1–O2	77.06 (7)	O2–Pr1–O6	127.72 (8)
O13 ⁱⁱ –Pr1–O1	74.17 (8)	O10 ⁱ –Pr1–O2	140.20 (7)	O3–Pr2–O8	67.83 (7)
O12 ⁱ –Pr1–O7	84.33 (8)	O13 ⁱⁱ –Pr1–O2	133.21 (7)	O3–Pr2–O9 ⁱⁱⁱ	131.37 (7)
O10 ⁱ –Pr1–O7	73.43 (8)	O1–Pr1–O2	64.99 (7)	O8–Pr2–O9 ⁱⁱⁱ	65.55 (7)
O13 ⁱⁱ –Pr1–O7	115.33 (8)	O7–Pr1–O2	73.82 (7)	O3–Pr2–O14 ^{iv}	82.05 (8)
O1–Pr1–O7	72.73 (8)	O5–Pr1–O2	73.00 (7)	O8–Pr2–O14 ^{iv}	74.36 (7)
O12 ⁱ –Pr1–O5	106.88 (7)	O12 ⁱ –Pr1–O6	75.20 (8)	O9 ⁱⁱⁱ –Pr2–O14 ^{iv}	73.01 (7)
O3–Pr2–O15	71.52 (8)	O9 ⁱⁱⁱ –Pr2–O11	86.14 (7)	O3–Pr2–N3	140.52 (7)
O8–Pr2–O15	125.31 (8)	O14 ^{iv} –Pr2–O11	144.56 (7)	O8–Pr2–N3	141.59 (7)
O9 ⁱⁱⁱ –Pr2–O15	128.31 (7)	O15–Pr2–O11	144.87 (7)	O9 ⁱⁱⁱ –Pr2–N3	78.02 (7)
O14 ^{iv} –Pr2–O15	65.07 (7)	N1–Pr2–O11	61.36 (8)	O14 ^{iv} –Pr2–N3	84.02 (8)
O3–Pr2–N1	137.53 (8)	O3–Pr2–O4	65.42 (7)	O15–Pr2–N3	69.10 (8)
O8–Pr2–N1	123.30 (8)	O8–Pr2–O4	120.68 (7)	N1–Pr2–N3	59.18 (8)
O9 ⁱⁱⁱ –Pr2–N1	81.84 (8)	O9 ⁱⁱⁱ –Pr2–O4	156.25 (7)	O11–Pr2–N3	119.91 (7)
O14 ^{iv} –Pr2–N1	139.13 (8)	O14 ^{iv} –Pr2–O4	130.19 (7)	O4–Pr2–N3	97.56 (8)
O15–Pr2–N1	111.38 (8)	O15–Pr2–O4	69.21 (7)	N1–Pr2–O4	76.04 (8)
O3–Pr2–O11	91.41 (8)	O11–Pr2–O4	75.81 (7)	O8–Pr2–O11	70.94 (7)

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

4

Nd1–O7 ⁱ	2.376 (2)	Nd1–O6 ⁱ	2.409 (2)	Nd1–O8 ⁱⁱ	2.436 (2)
Nd1–O1	2.462 (2)	Nd1–O15	2.469 (2)	Nd1–O13	2.488 (2)
Nd1–O2	2.511 (2)	Nd1–O14	2.557 (2)	Nd2–O4	2.458 (2)
Nd2–O9	2.472 (2)	Nd2–O10 ⁱⁱⁱ	2.483 (2)	Nd2–O12 ^{iv}	2.486 (2)
Nd2–N1	2.494 (3)	Nd2–O11	2.497 (2)	Nd2–O5	2.528 (2)
Nd2–O3	2.535 (2)	Nd2–N3	2.838 (3)		
O7 ⁱ –Nd1–O6 ⁱ	78.29 (8)	O6 ⁱ –Nd1–O1	123.43 (8)	O8 ⁱⁱ –Nd1–O15	115.09 (9)
O7 ⁱ –Nd1–O8 ⁱⁱ	146.00 (8)	O8 ⁱⁱ –Nd1–O1	74.10 (8)	O1–Nd1–O15	72.82 (8)
O6 ⁱ –Nd1–O8 ⁱⁱ	81.33 (8)	O7 ⁱ –Nd1–O15	84.51 (8)	O7 ⁱ –Nd1–O13	106.19 (8)
O7 ⁱ –Nd1–O1	139.87 (8)	O6 ⁱ –Nd1–O15	73.15 (9)	O6 ⁱ –Nd1–O13	144.27 (8)
O8 ⁱⁱ –Nd1–O13	76.12 (8)	O8 ⁱⁱ –Nd1–O2	133.63 (8)	O6 ⁱ –Nd1–O14	73.25 (8)
O1–Nd1–O13	76.26 (8)	O1–Nd1–O2	65.44 (8)	O8 ⁱⁱ –Nd1–O14	73.03 (8)
O15–Nd1–O13	141.90 (9)	O15–Nd1–O2	74.02 (9)	O1–Nd1–O14	139.75 (8)
O7 ⁱ –Nd1–O2	76.81 (8)	O13–Nd1–O2	73.20 (8)	O15–Nd1–O14	143.53 (8)
O6 ⁱ –Nd1–O2	140.23 (8)	O7 ⁱ –Nd1–O14	75.17 (8)	O13–Nd1–O14	73.84 (8)
O2–Nd1–O14	127.98 (8)	O4–Nd2–O9	67.61 (8)	O4–Nd2–O10 ⁱⁱⁱ	131.50 (8)
O9–Nd2–O10 ⁱⁱⁱ	65.79 (7)	N1–Nd2–O11	110.92 (9)	O11–Nd2–O5	144.47 (7)
O4–Nd2–O12 ^{iv}	82.32 (8)	O9–Nd2–O5	71.07 (8)	O4–Nd2–O3	65.77 (8)
O9–Nd2–O12 ^{iv}	74.32 (8)	O10 ⁱⁱⁱ –Nd2–O5	86.17 (8)	O9–Nd2–O3	120.92 (7)
O10 ⁱⁱⁱ –Nd2–O12 ^{iv}	73.05 (8)	O12 ^{iv} –Nd2–O5	144.61 (8)	O10 ⁱⁱⁱ –Nd2–O3	155.78 (7)
O4–Nd2–N1	137.50 (8)	N1–Nd2–O5	61.74 (8)	O12 ^{iv} –Nd2–O3	130.51 (7)
O9–Nd2–N1	123.81 (8)	O11–Nd2–O3	68.99 (7)	N1–Nd2–O3	75.58 (8)
O5–Nd2–O3	75.65 (7)	O10 ⁱⁱⁱ –Nd2–N3	77.98 (8)	O11–Nd2–N3	68.85 (8)
O4–Nd2–N3	140.33 (8)	O12 ^{iv} –Nd2–N3	83.46 (8)	O5–Nd2–N3	120.46 (8)

O9–Nd2–N3	141.55 (8)	N1–Nd2–N3	59.36 (8)	O3–Nd2–N3	97.40 (8)
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Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

5

Sm1–O7 ⁱ	2.345 (3)	Sm1–O6 ⁱ	2.376 (3)	Sm1–O8 ⁱⁱ	2.402 (3)
Sm1–O15	2.424 (3)	Sm1–O1	2.429 (3)	Sm1–O13	2.462 (3)
Sm1–O2	2.490 (2)	Sm1–O14	2.518 (3)		
Sm2–O4	2.429 (2)	Sm2–O10 ⁱⁱⁱ	2.454 (2)	Sm2–O12 ^{iv}	2.463 (2)
Sm2–O9	2.472 (2)	Sm2–N1	2.476 (3)	Sm2–O11	2.480 (2)
Sm2–O5	2.505 (2)	Sm2–O3	2.507 (3)	Sm2–N3	2.845 (3)
O7 ⁱ –Sm1–O6 ⁱ	79.06 (10)	O7 ⁱ –Sm1–O13	103.66(11)	O13–Sm1–O2	73.67 (11)
O7 ⁱ –Sm1–O8 ⁱⁱ	145.38 (10)	O6 ⁱ –Sm1–O13	142.84(11)	O7 ⁱ –Sm1–O14	74.60 (11)
O6 ⁱ –Sm1–O8 ⁱⁱ	80.53 (10)	O8 ⁱⁱ –Sm1–O13	77.18 (11)	O6 ⁱ –Sm1–O14	72.53 (10)
O7 ⁱ –Sm1–O15	85.10 (11)	O15–Sm1–O13	144.07(12)	O8 ⁱⁱ –Sm1–O14	72.74 (11)
O6 ⁱ –Sm1–O15	72.74 (12)	O1–Sm1–O13	77.72 (12)	O15–Sm1–O14	142.40 (12)
O8 ⁱⁱ –Sm1–O15	114.87 (11)	O7 ⁱ –Sm1–O2	76.34 (9)	O1–Sm1–O14	139.41 (11)
O7 ⁱ –Sm1–O1	140.36 (9)	O6 ⁱ –Sm1–O2	140.52(11)	O13–Sm1–O14	72.63 (11)
O6 ⁱ –Sm1–O1	123.76 (10)	O8 ⁱⁱ –Sm1–O2	134.39(10)	O2–Sm1–O14	128.02 (10)
O8 ⁱⁱ –Sm1–O1	74.14 (10)	O15–Sm1–O2	74.82 (12)	O1–Sm1–O2	65.95 (9)
O15–Sm1–O1	73.99 (12)	O4–Sm2–O10 ⁱⁱⁱ	131.78 (9)	O4–Sm2–O12 ^{iv}	81.26 (11)
O10 ⁱⁱⁱ –Sm2–O12 ^v	73.33 (9)	O12 ^{iv} –Sm2–O11	65.65 (9)	O10 ⁱⁱⁱ –Sm2–O3	155.38 (8)
O4–Sm2–O9	67.69 (9)	N1–Sm2–O11	109.97(10)	O9–Sm2–O3	120.40 (10)
O10 ⁱⁱⁱ –Sm2–O9	66.28 (9)	O4–Sm2–O5	92.11 (10)	N1–Sm2–O3	75.76 (10)
O12 ^{iv} –Sm2–O9	74.27 (10)	O10 ⁱⁱⁱ –Sm2–O5	86.33 (10)	O11–Sm2–O3	69.35 (9)
O4–Sm2–N1	138.62 (11)	O12 ^{iv} –Sm2–O5	144.74 (9)	O5–Sm2–O3	75.06 (10)
O10 ⁱⁱⁱ –Sm2–N1	81.37 (9)	O9–Sm2–O5	71.21 (9)	O4–Sm2–N3	139.43 (10)
O12 ^{iv} –Sm2–N1	138.55 (10)	N1–Sm2–O5	62.11 (9)	O10 ⁱⁱⁱ –Sm2–N3	77.54 (9)
O9–Sm2–N1	124.16 (10)	O11–Sm2–O5	144.32(10)	O12 ^{iv} –Sm2–N3	83.12 (10)
O4–Sm2–O11	71.45 (10)	O4–Sm2–O3	66.07 (10)	O9–Sm2–N3	141.39 (9)
O10 ⁱⁱⁱ –Sm2–O11	128.40 (10)	O5–Sm2–N3	120.84 (9)	N1–Sm2–N3	59.36 (9)
O11–Sm2–N3	67.99 (9)	O3–Sm2–N3	98.10 (10)		

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

6

Eu1–O14 ⁱ	2.320 (4)	Eu1–O1	2.427 (4)	Eu1–O2	2.483 (4)
Eu1–O13 ⁱ	2.373 (3)	Eu1–O5	2.429 (4)	Eu1–O6	2.539 (4)
Eu1–O15 ⁱⁱ	2.378 (3)	Eu1–O7	2.455 (3)		
Eu2–O4	2.427 (4)	Eu2–N2	2.459 (4)	Eu2–N1	2.852 (5)
Eu2–O8	2.440 (4)	Eu2–O11 ^{iv}	2.476 (4)	Eu2–O3	2.519 (3)
Eu2–O9 ⁱⁱⁱ	2.443 (3)	Eu2–O12	2.498 (3)	Eu2–O10	2.454 (4)
O14 ⁱ –Eu1–O13 ⁱ	79.55 (12)	O7–Eu1–O2	73.32 (12)	O9 ⁱⁱⁱ –Eu2–O12	86.25 (12)
O14 ⁱ –Eu1–O15 ⁱⁱ	145.88 (13)	O14 ⁱ –Eu1–O6	75.28 (13)	N2–Eu2–N1	59.43 (13)
O13 ⁱ –Eu1–O15 ⁱⁱ	80.40 (12)	O13 ⁱ –Eu1–O6	72.77 (12)	O11 ^{iv} –Eu2–N1	67.88 (12)
O14 ⁱ –Eu1–O1	140.61 (12)	O15 ⁱⁱ –Eu1–O6	72.54 (13)	O12–Eu2–N1	121.55 (12)
O13 ⁱ –Eu1–O1	122.77 (12)	O1–Eu1–O6	138.92(12)	O3–Eu2–N1	96.80 (13)
O15 ⁱⁱ –Eu1–O1	73.43 (12)	O5–Eu1–O6	142.94(12)	O10–Eu2–O12	144.51 (12)
O14 ⁱ –Eu1–O5	85.61 (13)	O7–Eu1–O6	73.41 (12)	N2–Eu2–O12	62.81 (12)
O13 ⁱ –Eu1–O5	72.71 (12)	O2–Eu1–O6	128.81(12)	O11 ^{iv} –Eu2–O12	143.73 (12)
O15 ⁱⁱ –Eu1–O5	114.13 (13)	O4–Eu2–O12	91.03 (12)	O4–Eu2–O3	66.47 (12)
O1–Eu1–O5	73.29 (13)	O8–Eu2–O12	70.95 (12)	O4–Eu2–N1	139.44 (12)
O14 ⁱ –Eu1–O7	103.81 (12)	O8–Eu2–O3	121.11(12)	O8–Eu2–N1	142.02 (12)
O13 ⁱ –Eu1–O7	143.82 (13)	O9 ⁱⁱⁱ –Eu2–O3	154.74(12)	O9 ⁱⁱⁱ –Eu2–N1	77.77 (12)
O15 ⁱⁱ –Eu1–O7	77.60 (12)	O10–Eu2–O3	130.63(12)	O10–Eu2–N1	83.05 (13)
O1–Eu1–O7	77.41 (12)	N2–Eu2–O3	74.42 (12)	O1–Eu1–O2	66.30 (12)
O5–Eu1–O7	142.97 (12)	O11 ^{iv} –Eu2–O3	68.38 (12)	O5–Eu1–O2	74.45 (12)
O14 ⁱ –Eu1–O2	76.27 (12)	O12–Eu2–O3	75.54 (12)	O15 ⁱⁱ –Eu1–O2	134.23 (12)
O13 ⁱ –Eu1–O2	140.29 (12)				

Symmetry codes: (i) $x-1, -y+3/2, z-1/2$; (ii) $x-1, y, z-1$; (iii) $-x+1, -y+1, -z$; (iv) $-x, -y+1, -z$; (v) $x+1, -y+3/2, z+1/2$; (vi) $x+1, y, z+1$.

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Gd1–O4	2.396 (36)	Gd1–O10 ⁱ	2.426 (3)	Gd1–O12 ⁱⁱ	2.434 (3)
Gd1–O9	2.443 (3)	Gd1–N1	2.445 (3)	Gd1–O11	2.456 (3)

Gd1–O5	2.475 (3)	Gd1–O3	2.494 (3)		
Gd2–O7 ⁱⁱⁱ	2.311 (3)	Gd2–O15	2.390 (3)	Gd2–O2	2.470 (3)
Gd2–O6 ⁱⁱⁱ	2.356 (3)	Gd2–O1	2.408 (3)	Gd2–O14	2.485 (3)
Gd2–O8 ^{iv}	2.373 (3)	Gd2–O13	2.422 (3)		
O4–Gd1–O10 ⁱ	132.07 (9)	O10 ⁱ –Gd1–O3	154.72 (9)	O6 ⁱⁱⁱ –Gd2–O1	123.48 (9)
O4–Gd1–O12 ⁱⁱ	81.68 (10)	O12 ⁱⁱ –Gd1–O3	131.17 (9)	O8 ^{iv} –Gd2–O1	73.96 (9)
O10 ⁱ –Gd1–O12 ⁱⁱ	73.35 (9)	O9–Gd1–O3	120.73 (9)	O15–Gd2–O1	74.17 (10)
O4–Gd1–O9	67.28 (9)	N1–Gd1–O3	74.78 (9)	O7 ⁱⁱⁱ –Gd2–O13	102.88 (10)
O10 ⁱ –Gd1–O9	66.81 (9)	O11–Gd1–O3	68.90 (9)	O6 ⁱⁱⁱ –Gd2–O13	142.45 (10)
O12 ⁱⁱ –Gd1–O9	74.09 (9)	O5–Gd1–O3	75.09 (9)	O8 ^{iv} –Gd2–O13	78.18 (10)
O4–Gd1–N1	138.22 (10)	O4–Gd1–N3	139.10 (9)	O15–Gd2–O13	144.75 (10)
O10 ⁱ –Gd1–N1	81.61 (9)	O10 ⁱ –Gd1–N3	77.66 (9)	O1–Gd2–O13	78.10 (10)
O12 ⁱⁱ –Gd1–N1	138.34 (10)	O12 ⁱⁱ –Gd1–N3	82.65 (10)	O7 ⁱⁱⁱ –Gd2–O2	75.78 (9)
O9–Gd1–N1	125.21 (9)	O9–Gd1–N3	141.69 (9)	O6 ⁱⁱⁱ –Gd2–O2	140.75 (10)
O4–Gd1–O11	71.86 (9)	N1–Gd1–N3	59.46 (9)	O8 ^{iv} –Gd2–O2	134.91 (9)
O10 ⁱ –Gd1–O11	128.77 (9)	O11–Gd1–N3	67.24 (9)	O15–Gd2–O2	75.34 (10)
O12 ⁱⁱ –Gd1–O11	66.38 (9)	O5–Gd1–N3	121.58 (9)	O1–Gd2–O2	66.24 (9)
O9–Gd1–O11	126.05 (9)	O3–Gd1–N3	97.52 (10)	O13–Gd2–O2	73.80 (10)
N1–Gd1–O11	108.71 (9)	O7 ⁱⁱⁱ –Gd2–O6 ⁱⁱⁱ	79.91 (9)	O7 ⁱⁱⁱ –Gd2–O14	74.36 (10)
O4–Gd1–O5	91.68 (9)	O7 ⁱⁱⁱ –Gd2–O8 ^{iv}	145.73 (10)	O6 ⁱⁱⁱ –Gd2–O14	72.28 (10)
O10 ⁱ –Gd1–O5	86.26 (9)	O6 ⁱⁱⁱ –Gd2–O8 ^{iv}	79.53 (10)	O8 ^{iv} –Gd2–O14	73.40 (10)
O12 ⁱⁱ –Gd1–O5	144.52 (9)	O7 ⁱⁱⁱ –Gd2–O15	85.51 (10)	O15–Gd2–O14	141.79 (10)
O9–Gd1–O5	71.23 (9)	O6 ⁱⁱⁱ –Gd2–O15	72.43 (10)	O1–Gd2–O14	139.67 (10)
N1–Gd1–O5	62.81 (9)	O8 ^{iv} –Gd2–O15	113.66 (9)	O13–Gd2–O14	72.59 (9)
O11–Gd1–O5	143.89 (9)	O7 ⁱⁱⁱ –Gd2–O1	140.22 (9)	O2–Gd2–O14	127.91 (9)
O4–Gd1–O3	66.54 (9)				

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

8

Tb1–O4	2.385 (3)	Tb1–O5	2.454 (3)	Tb2–O15	2.373 (3)
Tb1–O10 ⁱ	2.410 (3)	Tb1–O3	2.487 (3)	Tb2–O1	2.391 (3)
Tb1–O12 ⁱⁱ	2.416 (3)	Tb2–O7 ⁱⁱⁱ	2.293 (3)	Tb2–O13	2.409 (3)
Tb1–N1	2.428 (3)	Tb2–O6 ⁱⁱⁱ	2.342 (3)	Tb2–O2	2.456 (3)
Tb1–O9	2.436 (3)	Tb2–O8 ^{iv}	2.354 (3)	Tb2–O14	2.470 (3)
Tb1–O11	2.444 (3)				
O4–Tb1–O10 ⁱ	132.55 (9)	O10 ⁱ –Tb1–O3	154.23 (9)	O8 ^{iv} –Tb2–O1	73.58 (10)
O4–Tb1–O12 ⁱⁱ	81.36 (10)	O12 ⁱⁱ –Tb1–O3	131.35 (9)	O15–Tb2–O1	74.33 (10)
O10 ⁱ –Tb1–O12 ⁱⁱ	73.60 (9)	N1–Tb1–O3	74.53 (9)	O7 ⁱⁱⁱ –Tb2–O13	102.77 (10)
O4–Tb1–N1	138.48 (10)	O9–Tb1–O3	120.87 (9)	O6 ⁱⁱⁱ –Tb2–O13	142.55 (10)
O10 ⁱ –Tb1–N1	81.38 (9)	O11–Tb1–O3	68.88 (9)	O8 ^{iv} –Tb2–O13	78.60 (10)
O12 ⁱⁱ –Tb1–N1	138.20 (10)	O5–Tb1–O3	74.97 (9)	O15–Tb2–O13	144.89 (10)
O4–Tb1–O9	67.48 (9)	O4–Tb1–N3	138.50 (10)	O1–Tb2–O13	78.06 (10)
O10 ⁱ –Tb1–O9	67.12 (9)	O10 ⁱ –Tb1–N3	77.50 (9)	O7 ⁱⁱⁱ –Tb2–O2	75.59 (9)
O12 ⁱⁱ –Tb1–O9	73.84 (9)	O12 ⁱⁱ –Tb1–N3	82.53 (10)	O6 ⁱⁱⁱ –Tb2–O2	140.79 (10)
N1–Tb1–O9	125.73 (10)	N1–Tb1–N3	59.36 (10)	O8 ^{iv} –Tb2–O2	135.03 (9)
O4–Tb1–O11	71.55 (10)	O9–Tb1–N3	141.61 (9)	O15–Tb2–O2	75.63 (10)
O10 ⁱ –Tb1–O11	128.87 (9)	O11–Tb1–N3	66.95 (9)	O1–Tb2–O2	66.54 (9)
O12 ⁱⁱ –Tb1–O11	66.59 (9)	O5–Tb1–N3	121.94 (9)	O13–Tb2–O2	73.72 (10)
N1–Tb1–O11	108.18 (10)	O3–Tb1–N3	97.47 (10)	O7 ⁱⁱⁱ –Tb2–O14	74.58 (10)
O9–Tb1–O11	126.07 (9)	O7 ⁱⁱⁱ –Tb2–O6 ⁱⁱⁱ	80.20 (9)	O6 ⁱⁱⁱ –Tb2–O14	72.26 (10)
O4–Tb1–O5	91.96 (10)	O7 ⁱⁱⁱ –Tb2–O8 ^{iv}	145.99 (10)	O8 ^{iv} –Tb2–O14	73.50 (10)
O10 ⁱ –Tb1–O5	86.22 (9)	O6 ⁱⁱⁱ –Tb2–O8 ^{iv}	79.20 (10)	O15–Tb2–O14	141.61 (10)
O12 ⁱⁱ –Tb1–O5	144.38 (9)	O7 ⁱⁱⁱ –Tb2–O15	85.62 (10)	O1–Tb2–O14	139.39 (10)
N1–Tb1–O5	63.28 (9)	O6 ⁱⁱⁱ –Tb2–O15	72.15 (10)	O13–Tb2–O14	72.71 (10)
O9–Tb1–O5	71.32 (9)	O8 ^{iv} –Tb2–O15	113.04 (10)	O2–Tb2–O14	128.04 (10)
O11–Tb1–O5	143.74 (9)	O7 ⁱⁱⁱ –Tb2–O1	140.36 (10)		
O4–Tb1–O3	66.73 (9)	O6 ⁱⁱⁱ –Tb2–O1	123.20 (9)		

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$; (vii) $x, -y+1/2, z+1/2$.

9

Dy1–O7 ⁱ	2.270 (3)	Dy1–O2	2.456 (3)	Dy2–O9	2.418 (3)
Dy1–O6 ⁱ	2.338 (3)	Dy1–O14	2.484 (3)	Dy2–O11	2.439 (3)
Dy1–O8 ⁱⁱⁱ	2.342 (3)	Dy2–O4	2.381 (3)	Dy2–O5	2.453 (3)
Dy1–O15	2.379 (3)	Dy2–O10 ⁱⁱⁱ	2.401 (3)	Dy2–O3	2.483 (3)

Dy1-O1	2.386 (3)	Dy2-O12 ^{iv}	2.405 (3)	Dy2-N3	2.810 (4)
Dy1-O13	2.406 (3)	Dy2-N1	2.416 (3)		
O7 ⁱ -Dy1-O6 ⁱ	80.96 (10)	O8 ⁱⁱ -Dy1-O2	134.53 (10)	O4-Dy2-O9	66.87 (10)
O7 ⁱ -Dy1-O8 ⁱⁱⁱ	146.72 (10)	O15-Dy1-O2	75.02 (10)	O10 ⁱⁱⁱ -Dy2-O9	67.76 (9)
O6 ⁱ -Dy1-O8 ⁱⁱ	79.24 (10)	O1-Dy1-O2	67.09 (10)	O12 ^{iv} -Dy2-O9	73.87 (10)
O7 ⁱ -Dy1-O15	85.08 (11)	O13-Dy1-O2	73.47 (11)	N1-Dy2-O9	125.42 (10)
O6 ⁱ -Dy1-O15	72.61 (11)	O7 ⁱ -Dy1-O14	75.55 (11)	O4-Dy2-O11	71.61 (10)
O8 ⁱⁱ -Dy1-O15	113.73 (10)	O6 ⁱ -Dy1-O14	72.31 (10)	O10 ⁱⁱⁱ -Dy2-O1	129.14 (10)
O7 ⁱ -Dy1-O1	140.29 (10)	O8 ⁱⁱ -Dy1-O14	73.07 (10)	O12 ^{iv} -Dy2-O1	67.02 (10)
O6 ⁱ -Dy1-O1	121.87 (10)	O15-Dy1-O14	142.04 (11)	N1-Dy2-O11	108.78 (10)
O8 ⁱⁱ -Dy1-O1	72.94 (10)	O1-Dy1-O14	139.17 (11)	O9-Dy2-O11	125.74 (10)
O15-Dy1-O1	73.72 (11)	O13-Dy1-O14	73.59 (11)	O4-Dy2-O5	90.74 (10)
O7 ⁱ -Dy1-O13	103.76 (11)	O2-Dy1-O14	128.53 (10)	O10 ⁱⁱⁱ -Dy2-O5	86.73 (10)
O6 ⁱ -Dy1-O13	143.10 (11)	O4-Dy2-O10 ⁱⁱⁱ	132.69 (9)	O12 ^{iv} -Dy2-O5	143.98 (10)
O8 ⁱⁱ -Dy1-O13	77.75 (11)	O4-Dy2-O12 ^{iv}	81.93 (11)	N1-Dy2-O5	63.62 (10)
O15-Dy1-O13	143.67 (11)	O10 ⁱⁱⁱ -Dy2-O ^v	73.35 (10)	O9-Dy2-O5	70.84 (10)
O1-Dy1-O13	77.68 (11)	O4-Dy2-N1	138.33 (11)	O11-Dy2-O5	143.13 (10)
O7 ⁱ -Dy1-O2	75.25 (10)	O10 ⁱⁱⁱ -Dy2-N1	80.88 (10)	O4-Dy2-O3	67.49 (10)
O6 ⁱ -Dy1-O2	141.08 (11)	O12 ^{iv} -Dy2-N1	138.09 (11)	O10 ⁱⁱⁱ -Dy2-O3	153.63 (9)
O12 ^{iv} -Dy2-O3	131.89 (10)	O5-Dy2-O3	74.94 (10)	N1-Dy2-N3	60.22 (10)
N1-Dy2-O3	74.07 (10)	O4-Dy2-N3	138.55 (10)	O9-Dy2-N3	141.79 (10)
O9-Dy2-O3	121.33 (10)	O10 ⁱⁱⁱ -Dy2-N3	77.30 (10)	O11-Dy2-N3	66.94 (10)
O11-Dy2-O3	68.46 (10)	O12 ^{iv} -Dy2-N3	81.92 (10)	O5-Dy2-N3	123.24 (9)
O3-Dy2-N3	96.85 (10)				

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

10

Ho1-O7 ⁱ	2.258 (3)	Ho1-O15	2.348 (3)	Ho1-O2	2.439 (3)
Ho1-O6 ⁱ	2.325 (3)	Ho1-O1	2.368 (3)	Ho1-O14	2.447 (3)
Ho1-O8 ⁱⁱ	2.330 (3)	Ho1-O13	2.374 (4)	Ho2-O5	2.428 (3)
Ho2-O4	2.356 (3)	Ho2-N1	2.406 (4)	Ho2-O3	2.470 (3)
Ho2-O10 ⁱⁱⁱ	2.386 (3)	Ho2-O9	2.416 (3)	Ho2-N3	2.854 (4)
Ho2-O12 ^{iv}	2.396 (3)	Ho2-O11	2.423 (3)		
O7 ⁱ -Ho1-O6 ⁱ	81.09 (11)	O13-Ho1-O2	73.77 (13)	O8 ⁱⁱ -Ho1-O14	73.52 (11)
O7 ⁱ -Ho1-O8 ⁱⁱ	146.03 (11)	O7 ⁱ -Ho1-O14	74.62 (12)	O15-Ho1-O14	141.43 (12)
O6 ⁱ -Ho1-O8 ⁱⁱⁱ	78.33 (11)	O6 ⁱ -Ho1-O14	72.26 (12)	O1-Ho1-O14	139.24 (12)
O7 ⁱ -Ho1-O15	85.89 (12)	O10 ⁱⁱⁱ -Ho2-O5	86.70 (11)	O13-Ho1-O14	72.58 (12)
O6 ⁱ -Ho1-O15	72.04 (12)	O12 ^{iv} -Ho2-O5	144.16(11)	O2-Ho1-O14	127.97 (11)
O8 ⁱⁱ -Ho1-O15	112.58 (11)	N1-Ho2-O5	63.81 (11)	O4-Ho2-O10 ⁱⁱⁱ	132.87 (10)
O7 ⁱ -Ho1-O1	140.38 (11)	O9-Ho2-O5	71.18 (11)	O4-Ho2-O12 ^{iv}	81.75 (12)
O6 ⁱ -Ho1-O1	122.72 (11)	O11-Ho2-O5	143.40(11)	O10 ⁱⁱⁱ -Ho2-O12 ^{iv}	73.13 (11)
O8 ⁱⁱ -Ho1-O1	73.50 (11)	O4-Ho2-O3	67.16 (11)	O4-Ho2-N1	138.51 (12)
O15-Ho1-O1	74.48 (12)	O10 ⁱⁱⁱ -Ho2-O3	153.78(10)	O10 ⁱⁱⁱ -Ho2-N1	81.29 (11)
O7 ⁱ -Ho1-O13	102.11 (12)	O12 ^{iv} -Ho2-O3	132.09(11)	O12 ^{iv} -Ho2-N1	137.75 (12)
O6 ⁱ -Ho1-O13	142.35 (13)	N1-Ho2-O3	74.03 (11)	O10 ⁱⁱⁱ -Ho2-O11	128.61 (11)
O8 ⁱⁱ -Ho1-O13	79.22 (12)	O9-Ho2-O3	121.12(11)	O12 ^{iv} -Ho2O11	67.25 (10)
O15-Ho1-O13	145.19 (13)	O11-Ho2-O3	68.85 (11)	O10 ⁱⁱⁱ -Ho2-O9	67.53 (10)
O1-Ho1-O13	78.31 (13)	O5-Ho2-O3	74.67 (11)	O12 ^{iv} -Ho2-O9	73.77 (11)
O7 ⁱ -Ho1-O2	75.07 (11)	O4-Ho2-N3	138.21(12)	O3-Ho2-N3	97.30 (11)
O6 ⁱ -Ho1-O2	141.00 (12)	O10 ⁱⁱⁱ -Ho2-N3	77.17 (11)	N1-Ho2-O9	126.01 (12)
O8 ⁱⁱ -Ho1-O2	135.56 (11)	O12 ^{iv} -Ho2-N3	81.99 (12)	O4-Ho2-O11	71.92 (11)
O15-Ho1-O2	75.83 (12)	N1-Ho2-N3	59.55 (11)	O4-Ho2-O9	67.44 (10)
O1-Ho1-O2	66.97 (11)	O9-Ho2-N3	141.54(11)	O11-Ho2-N3	66.30 (11)
O9-Ho2-O11	126.53 (11)	N1-Ho2-O11	107.44(11)	O5-Ho2-N3	122.68 (10)
O4-Ho2-O5	91.58 (11)				

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

11

Er1-O7 ⁱ	2.246 (3)	Er1-O15	2.332 (4)	Er1-O14	2.435 (4)
Er1-O8 ⁱⁱ	2.319 (3)	Er1-O13	2.364 (4)	Er1-O2	2.438 (3)
Er1-O6 ⁱ	2.321 (3)	Er1-O1	2.366 (3)	Er2-O4	2.351 (3)
Er2-O10 ⁱⁱⁱ	2.380 (3)	Er2-O9	2.411 (3)	Er2-O3	2.468 (3)
Er2-O12 ^{iv}	2.387 (3)	Er2-O11	2.414 (3)	Er2-N3	2.861 (5)
Er2-N1	2.401 (4)	Er2-O5	2.419 (3)		

O7 ⁱ –Er1–O8 ⁱⁱ	146.38 (12)	O6 ⁱ –Er1–O14	72.12 (13)	O4–Er2–O9	67.35 (11)
O7 ⁱ –Er1–O6 ⁱ	81.40 (12)	O15–Er1–O14	141.13(13)	O10 ⁱⁱⁱ –Er2–O9	67.68 (11)
O8 ⁱⁱ –Er1–O6 ⁱ	78.23 (12)	O13–Er1–O14	72.69 (13)	O12 ^{iv} –Er2–O9	73.57 (12)
O7 ⁱ –Er1–O15	86.03 (13)	O1–Er1–O14	139.31(13)	N1–Er2–O9	126.51 (12)
O8 ⁱⁱ –Er1–O15	112.17 (13)	O7 ⁱ –Er1–O2	74.74 (11)	O4–Er2–O11	71.97 (12)
O6 ⁱ –Er1–O15	71.84 (13)	O8 ⁱⁱ –Er1–O2	135.61(12)	O10 ⁱⁱⁱ –Er2–O11	128.90 (12)
O7 ⁱ –Er1–O13	101.69 (14)	O6 ⁱ –Er1–O2	140.97(12)	O12 ^{iv} –Er2–O11	67.78 (11)
O8 ⁱⁱ –Er1–O13	79.60 (14)	O15–Er1–O2	76.05 (13)	N1–Er2–O11	106.74 (13)
O6 ⁱ –Er1–O13	142.38 (14)	O13–Er1–O2	73.69 (14)	O9–Er2–O11	126.72 (12)
O15–Er1–O13	145.38 (14)	O1–Er1–O2	67.14 (12)	O4–Er2–O5	91.48 (12)
O7 ⁱ –Er1–O1	140.25 (12)	O14–Er1–O2	128.02(13)	O10 ⁱⁱⁱ –Er2–O5	86.63 (12)
O8 ⁱⁱ –Er1–O1	73.28 (12)	O4–Er2–O10 ⁱⁱⁱ	132.97(11)	O12 ^{iv} –Er2–O5	143.88 (12)
O6 ⁱ –Er1–O1	122.62 (12)	O4–Er2–O12 ^{iv}	81.74 (13)	N1–Er2–O5	64.41 (12)
O15–Er1–O1	74.54 (13)	O10 ⁱⁱⁱ –Er2–O12 ^{iv}	73.13 (11)	O9–Er2–O5	71.11 (11)
O13–Er1–O1	78.49 (13)	O4–Er2–N1	138.68(12)	O11–Er2–O5	143.11 (11)
O7 ⁱ –Er1–O14	74.67 (13)	O10 ⁱⁱⁱ –Er2–N1	81.24 (12)	O4–Er2–O3	67.34 (12)
O8 ⁱⁱ –Er1–O14	73.74 (13)	O12 ^{iv} –Er2–N1	137.47(13)	O10 ⁱⁱⁱ –Er2–O3	153.50 (11)
O12 ^{iv} –Er2–O3	132.34 (11)	O5–Er2–O3	74.66 (12)	N1–Er2–N3	59.44 (12)
N1–Er2–O3	73.85 (12)	O4–Er2–N3	137.99(12)	O9–Er2–N3	141.47 (12)
O9–Er2–O3	121.20 (12)	O10 ⁱⁱⁱ –Er2–N3	77.15 (12)	O11–Er2–N3	66.03 (12)
O11–Er2–O3	68.57 (11)	O12 ^{iv} –Er2–N3	81.79 (13)	O5–Er2–N3	123.14 (11)
O3–Er2–N3	97.31 (13)				

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (ii) $x+1, y, z+1$; (iii) $-x+1, -y+1, -z+2$; (iv) $-x+2, -y+1, -z+2$; (v) $x-1, -y+1/2, z-1/2$; (vi) $x-1, y, z-1$.

Table S2. Hydrogen Bonds for 1-11 [Å and deg.]

D–H...A	D–H	H...A	D...A	D–H...A
1				
N3–H3A...O6 ^{iv}	0.86	2.11	2.966 (4)	174
Symmetry code: (iv) $x, y, z-1$.				
2				
O7–H7A...O5 ^{vi}	0.86 (5)	1.99 (5)	2.788 (3)	152 (5)
O7–H7B...O3 ⁱ	0.82 (5)	2.40 (6)	2.803 (4)	111 (5)
N3–H3A...O6 ^{iv}	0.86	2.08	2.938 (3)	177
Symmetry codes: (i) $x-1/2, -y+1/2, z+1/2$; (iv) $x, y, z-1$; (vi) $-x, -y, -z+2$.				
3				
N2–H2...O9 ^{vii}	0.88	2.07	2.845 (3)	147
O5–H5A...O14	0.81	2.04	2.808 (3)	157
O5–H5A...O15	0.81	2.65	3.361 (3)	147
O5–H5B...O11 ^{viii}	0.82	2.00	2.798 (3)	164
O6–H6A...O17 ⁱ	0.89	2.17	3.054 (5)	171
O6–H6B...O11 ^{viii}	0.89	1.85	2.737 (3)	173
O7–H7A...O16 ^{ix}	0.75	2.13	2.846 (4)	158
O7–H7B...O2 ^x	0.84	1.92	2.713 (3)	158
O16–H16B...O6 ^{vi}	0.82 (1)	2.65 (5)	2.931 (4)	102 (4)
O16–H16A...O4 ^{xi}	0.82 (1)	2.16 (2)	2.940 (3)	159 (4)
O17–H17B...O3 ^{xi}	0.83	2.26	2.912 (4)	135
O17–H17A...N2 ^x	0.80	2.46	3.092 (5)	136
O17–H17A...O16 ^{ix}	0.80	2.42	2.818 (4)	112
Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (vi) $x-1, y, z-1$; (vii) $x, y, z-1$; (viii) $x+1, y, z$; (ix) $x, y, z+1$; (x) $x, -y+1/2, z+1/2$; (xi) $x, -y+1/2, z-1/2$.				
4				
N2–H2...O10 ^{vii}	0.86	2.06	2.859 (3)	154
O13–H13A...O12	0.82	2.00	2.809 (3)	171
O13–H13B...O5 ^{viii}	0.82	2.02	2.799 (3)	157
O14–H14A...O16 ⁱ	0.82	2.19	2.990 (4)	167
O14–H14B...O5 ^{viii}	0.82	1.92	2.736 (3)	171
O15–H15A...O17 ^{ix}	0.82	2.05	2.831 (3)	159
O15–H15B...O2 ^x	0.82	1.90	2.716 (3)	172
O16–H16B...O4 ^{xi}	0.82	2.13	2.909 (4)	159
O16–H16A...O17 ^{ix}	0.82	2.11	2.824 (4)	145

O17–H17B...O14 ^{vi}	0.82	2.14	2.960 (3)	177
O17–H17A...O3 ^{xi}	0.82	2.10	2.919 (3)	176

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (vi) $x-1, y, z-1$; (vii) $x, y, z-1$; (viii) $x+1, y, z$; (ix) $x, y, z+1$; (x) $x, -y+1/2, z+1/2$; (xi) $x, -y+1/2, z-1/2$.

5

O15–H15B...O2 ^{vii}	0.82	1.94	2.734 (4)	163
O15–H15A...O17 ^{viii}	0.82	1.99	2.783 (6)	162
O14–H14B...O5 ^{ix}	0.82	2.01	2.752 (4)	150
O14–H14A...O16 ⁱ	0.82	2.14	2.916 (8)	159
O13–H13B...O5 ^{ix}	0.82	2.13	2.847 (4)	145
O13–H13A...O12	0.82	2.04	2.817 (4)	158
O13–H13A...O11	0.82	2.61	3.322 (4)	146
N2–H2...O10 ^x	0.86	2.17	2.928 (4)	146

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (vii) $x, -y+1/2, z+1/2$; (viii) $x, y, z+1$; (ix) $x+1, y, z$; (x) $x, y, z-1$.

6

O17–H17B...O6 ^{iv}	0.82 (1)	2.23 (1)	3.045 (5)	176 (6)
O17–H17A...O3 ^{vii}	0.82 (1)	2.05 (1)	2.863 (4)	173 (5)
O16–H16B...O17 ^{viii}	0.82 (1)	2.12 (3)	2.884 (5)	155 (6)
O16–H16A...O4 ⁱⁱⁱ	0.82 (1)	2.11 (3)	2.875 (5)	156 (6)
O7–H7B...O12 ^{ix}	0.82	2.07	2.806 (4)	150
O7–H7A...O10 ^{iv}	0.82	1.99	2.801 (4)	172
O6–H6B...O12 ^{ix}	0.82	2.00	2.747 (4)	152
O6–H6A...O16 ^{iv}	0.82	1.94	2.759 (5)	172
O5–H5B...O17 ⁱⁱⁱ	0.82	2.06	2.816 (5)	153
O5–H5A...O2 ^x	0.82	1.92	2.736 (4)	172
N3–H3...O9 ^{xi}	0.86	2.09	2.906 (4)	159

Symmetry codes: (iii) $-x+1, -y+1, -z$; (iv) $-x, -y+1, -z$; (vii) $-x+1, y-1/2, -z+1/2$; (viii) $x, -y+1/2, z+1/2$; (ix) $x-1, y, z$; (x) $x, -y+3/2, z-1/2$; (xi) $x, y, z+1$.

7

O17–H17A...O16 ^{vii}	0.82 (1)	2.25 (5)	2.865 (9)	132 (6)
O16–H16A...O4 ^{viii}	0.82 (1)	2.33 (9)	2.864 (7)	123 (9)
O15–H15B...O2 ^{ix}	0.82 (1)	1.93 (2)	2.741 (4)	168 (4)
O15–H15A...O17 ^x	0.82 (1)	1.99 (2)	2.778 (6)	160 (4)
O14–H14B...O5 ^{xi}	0.82 (1)	1.97 (2)	2.761 (4)	163 (5)
O14–H14A...O16 ⁱⁱⁱ	0.82 (1)	2.13 (2)	2.931 (8)	169 (4)
O13–H13B...O5 ^{xi}	0.82 (1)	2.04 (2)	2.833 (4)	163 (4)
O13–H13A...O12	0.82 (1)	2.01 (1)	2.823 (4)	174 (5)
N2–H2...O10 ^{vii}	0.86	2.38	2.947 (4)	123

Symmetry codes: (iii) $x+1, -y+1/2, z+1/2$; (vii) $x, y, z-1$; (viii) $x, -y+1/2, z-1/2$; (ix) $x, -y+1/2, z+1/2$; (x) $x, y, z+1$; (xi) $x+1, y, z$.

8

O15–H15B...O2 ^{vii}	0.82	1.93	2.743 (4)	168
O15–H15A...O17 ^{viii}	0.82	2.00	2.775 (6)	157
O14–H14B...O5 ^{ix}	0.82	1.97	2.766 (4)	164
O14–H14A...O16 ⁱⁱⁱ	0.82	2.11	2.918 (7)	173
O13–H13B...O5 ^{ix}	0.82	2.06	2.833 (4)	157
O13–H13A...O12	0.82	2.01	2.829 (4)	173
N2–H2...O10 ^x	0.86	2.20	2.956 (4)	146
N2–H2...O8	0.86	2.50	2.707 (4)	94

Symmetry codes: (iii) $x+1, -y+1/2, z+1/2$; (vii) $x, -y+1/2, z+1/2$; (viii) $x, y, z+1$; (ix) $x+1, y, z$; (x) $x, y, z-1$.

9

O17–H17B...O3 ^{vii}	0.82	2.12	2.838 (4)	145
O17–H17A...O14 ^{vi}	0.82	2.33	3.009 (4)	141
O16–H16B...O17 ^{viii}	0.82	2.12	2.852 (5)	148
O16–H16A...O4 ^{vii}	0.82	2.13	2.862 (4)	149
O15–H15B...O2 ^{ix}	0.82	1.90	2.716 (4)	173
O15–H15A...O17 ^{viii}	0.82	2.05	2.798 (4)	151
O14–H14B...O5 ^x	0.82	1.92	2.742 (4)	179
O14–H14A...O16 ⁱ	0.82	1.98	2.756 (5)	159
O13–H13B...O5 ^x	0.82	2.01	2.791 (4)	159
O13–H13A...O12	0.82	1.99	2.814 (4)	178
N2–H2...O10 ^{xi}	0.85	2.12	2.910 (4)	155

Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (vi) $x-1, y, z-1$; (vii) $x, -y+1/2, z-1/2$; (viii) $x, y, z+1$; (ix) $x, -y+1/2, z+1/2$; (x) $x+1, y, z$; (xi) $x, y, z-1$.

10

N2–H2...O10 ^{vii}	0.85	2.17	2.969 (4)	157
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O13–H13A···O12	0.82	2.02	2.834 (4)	176
O13–H13B···O5 ^{viii}	0.82	2.04	2.828 (4)	162
O14–H14A···O16 ⁱ	0.82	2.12	2.905 (7)	162
O14–H14B···O5 ^{viii}	0.82	1.96	2.762 (4)	165
O15–H15A···O17 ^{ix}	0.82	1.96	2.750 (6)	161
O15–H15B···O2 ^x	0.82	1.94	2.747 (4)	166
Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (vii) $x, y, z-1$; (viii) $x+1, y, z$; (ix) $x, y, z+1$; (x) $x, -y+1/2, z+1/2$.				
11				
O15–H15B···O2 ^{vii}	0.82	1.94	2.748 (5)	168
O15–H15A···O17 ^{viii}	0.82	1.97	2.747 (7)	157
O14–H14B···O5 ^{ix}	0.82	1.95	2.766 (5)	170
O14–H14A···O16 ⁱ	0.82	2.10	2.910 (8)	167
O13–H13B···O5 ^{ix}	0.82	2.02	2.825 (5)	169
O13–H13A···O12	0.82	2.04	2.841 (5)	167
N2–H2···O10 ^x	0.86	2.22	2.985 (5)	149
Symmetry codes: (i) $x+1, -y+1/2, z+1/2$; (vii) $x, -y+1/2, z+1/2$; (viii) $x, y, z+1$; (ix) $x+1, y, z$; (x) $x, y, z-1$				

Table S3 Preparation of **1** – **11**

Complex	Recipe (mmol for reagents and mL for solvents)							Product		
	Metal salt		H ₃ PIDC	H ₂ C ₂ O ₄	NaOH	H ₂ O	Ethanol	Formula	Colour	Yield
1	La(NO ₃) ₃ ·6H ₂ O	0.1	0.1	0.05	0.1	5.0	5.0	C ₁₁ H ₇ LaN ₃ O ₇	Yellow	55.3%
2	Ce(NO ₃) ₃ ·6H ₂ O	0.1	0.1	0.05	0.1	5.0	5.0	C ₁₁ H ₇ CeN ₃ O ₇	Yellow	60.2%
3	PrCl ₃ ·7H ₂ O	0.2	0.1	0.05	0.1	5.0	5.0	C ₁₄ H ₁₅ Pr ₂ N ₃ O ₁₇	Green	52.8%
4	NdCl ₃ ·6H ₂ O	0.2	0.1	0.05	0.1	5.0	5.0	C ₁₄ H ₁₅ Nd ₂ N ₃ O ₁₇	Purple	58.9%
5	SmCl ₃	0.2	0.1	0.05	0.1	5.0	5.0	C ₁₄ H ₁₅ Sm ₂ N ₃ O ₁₇	Yellow	62.5%
6	EuCl ₃	0.1	0.05	0.05	0	5.0	5.0	C ₁₄ H ₁₅ Eu ₂ N ₃ O ₁₇	Yellow	59.1%
7	GdCl ₃ ·6H ₂ O	0.1	0.05	0.05	0	5.0	5.0	C ₁₄ H ₁₅ Gd ₂ N ₃ O ₁₇	Yellow	52.9%
8	TbCl ₃ ·6H ₂ O	0.1	0.05	0.05	0	5.0	5.0	C ₁₄ H ₁₅ Tb ₂ N ₃ O ₁₇	Yellow	57.5%
9	DyCl ₃ ·6H ₂ O	0.2	0.1	0.1	0	5.0	5.0	C ₁₄ H ₁₅ Dy ₂ N ₃ O ₁₇	Yellow	53.4%
10	HoCl ₃ ·6H ₂ O	0.2	0.1	0.1	0	5.0	5.0	C ₁₄ H ₁₅ Ho ₂ N ₃ O ₁₇	Pink	66.4%
11	ErCl ₃ ·6H ₂ O	0.2	0.1	0.1	0	5.0	5.0	C ₁₄ H ₁₅ Er ₂ N ₃ O ₁₇	Pink	65.3%

Table S4 Elemental analysis and IR results of complexes **1** – **11**

	MW	Calcd / Found (%)			IR (KBr, cm ⁻¹)
		C	H	N	
1	432.09	30.58/30.54	1.63/1.61	9.72/9.76	3424w, 3169w, 1690m, 1625s, 1604s, 1534w, 1487m, 1450m, 1350m, 793m, 704w.
2	433.31	30.49/30.53	1.63/1.60	9.70/9.73	3427w, 3209w, 1666m, 1632s, 1589s, 1485w, 1443m, 1349m, 1310m, 801m, 702w
3	779.09	21.58/21.53	1.94/1.98	5.39/5.37	3424w, 3169w, 1690m, 1604s, 1534m, 1450w, 1310m, 1122m, 865m, 793m, 704w.
4	785.76	21.40/21.37	1.92/1.95	5.35/5.31	3420w, 3248w, 1692m, 1602s, 1533m, 1448w, 1310m, 1121m, 865m, 793m, 704w
5	798.00	21.07/21.01	1.89/1.93	5.27/5.33	3417w, 3206w, 1698m, 1622s, 1535m, 1485w, 1314m, 1124m, 797m, 744m, 708w
6	801.21	20.99/20.90	1.89/1.93	5.24/5.25	3210m, 1697w, 1621s, 1535m, 1485m, 1446w, 1314m, 1123m, 797m, 744w, 708m
7	811.78	20.71/20.69	1.86/1.83	5.18/5.15	3212w, 1699m, 1621s, 1536m, 1485w, 1445m, 1314m, 1124m, 796m, 707w.
8	815.13	20.63/20.70	1.85/1.82	5.16/5.19	3214w, 1702m, 1621s, 1537m, 1485w, 1446m, 1315m, 1124m, 797m, 708w.

9	822.28	20.45/20.39	1.84/1.83	5.11/5.16	3179w, 1701m, 1624s, 1536m, 1485w, 1446m, 1367m, 1155m, 796m, 708w.
10	826.90	20.33/20.37	1.83/1.88	5.08/5.02	3396w, 3180w, 1702m, 1625s, 1537m, 1486w, 1446m, 1315m, 1125m, 797m, 708w.
11	831.80	20.22/20.20	1.82/1.86	5.05/5.08	3394w, 1703m, 1625s, 1537m, 1486w, 1446m, 1315m, 1125m, 797m, 708w.

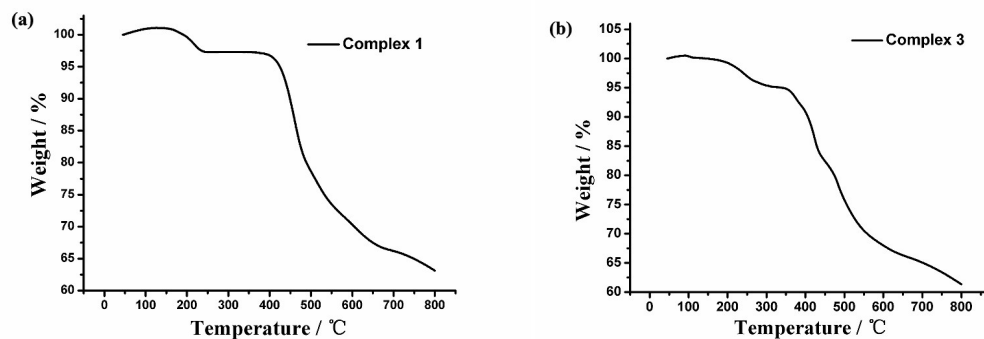


Fig. S1 TGA curves for complexes 1 and 3.

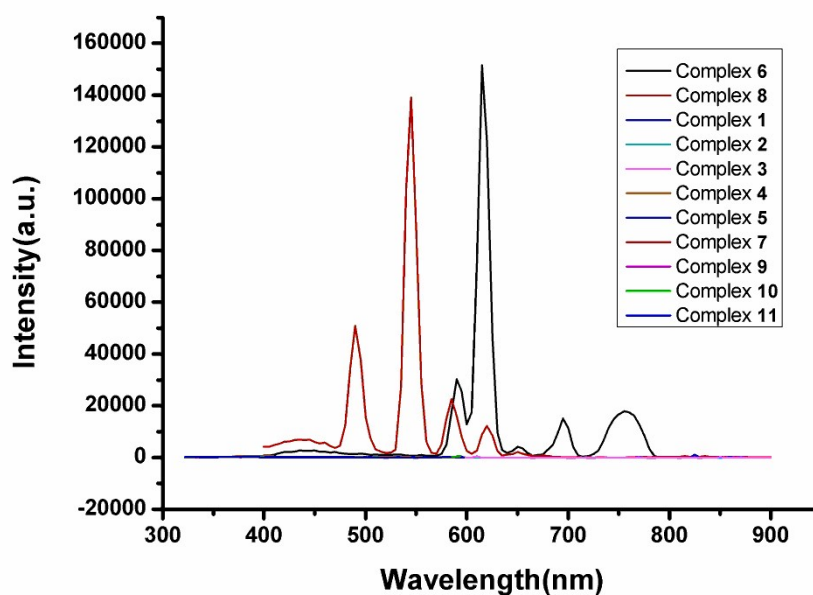
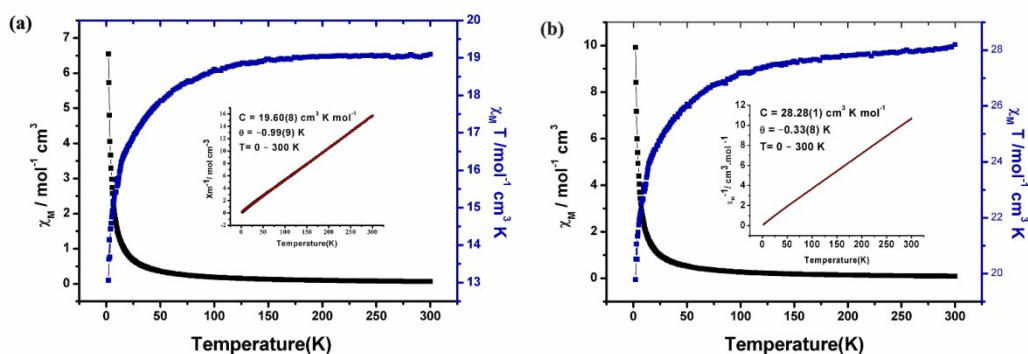


Fig. S2 The solid-state luminescent spectra of complexes 1-11.



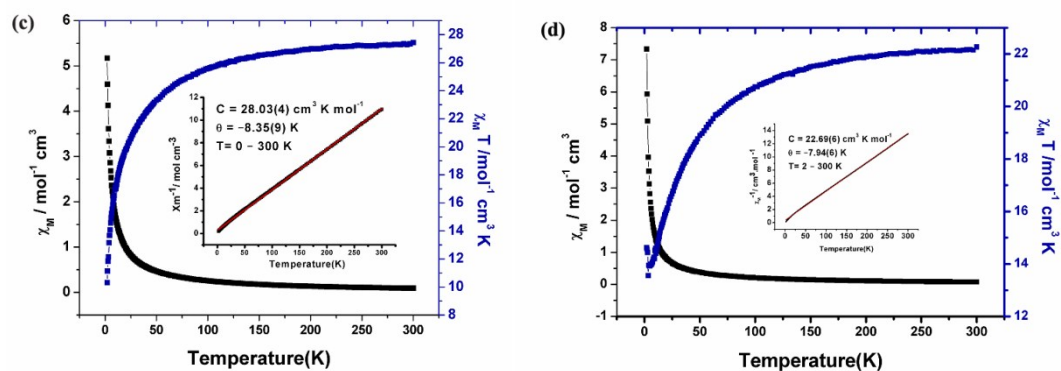


Fig.S3 Plots of χ_M (left), $\chi_M T$ (right) and χ_M^{-1} (insert) vs T for Ln(III) in 8-11