Electronic supplementary information

A series of lanthanide-transition metal coordination polymers with mixed ligands: syntheses, structures, photoluminescence and magnetic properties

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| Compound 1 ^{<i>a</i>} | | | | | |
|--------------------------------|----------|-----------------------------------|------------|--|------------|
| Co(1)-O(3) | 1.949(4) | N(3)-Co(1)-N(4) | 76.46(17) | O(9)-Y(1)-O(5) | 122.45(10) |
| Co(1)-N(1) | 2.050(4) | N(2)-Co(1)-N(4) | 76.17(18) | O(2)-Y(2)-O(8) ^{#2} | 76.43(13) |
| Co(1)-N(3) | 2.053(4) | O(16) ^{#1} -Y(1)-O(1) | 101.79(14) | O(2)-Y(2)-O(15) ^{#2} | 146.28(12) |
| Co(1)-N(2) | 2.072(5) | $O(16)^{\#1}$ -Y(1)-O(7) $^{\#2}$ | 76.90(13) | O(8) ^{#2} -Y(2)-O(15) ^{#2} | 74.70(12) |
| Co(1)-N(4) | 2.238(4) | O(1)-Y(1)-O(7) ^{#2} | 81.48(13) | O(2)-Y(2)-O(5) | 85.92(11) |
| Y(1)-O(16) ^{#1} | 2.227(3) | O(16) ^{#1} -Y(1)-O(10) | 81.25(13) | O(8) ^{#2} -Y(2)-O(5) | 87.31(11) |
| Y(1)-O(1) | 2.236(3) | O(1)-Y(1)-O(10) | 73.98(12) | O(15) ^{#2} -Y(2)-O(5) | 75.72(11) |
| Y(1)-O(7) ^{#2} | 2.294(3) | O(7) ^{#2} -Y(1)-O(10) | 142.83(13) | O(2)-Y(2)-O(13) | 130.77(12) |
| Y(1)-O(10) | 2.324(3) | O(16) ^{#1} -Y(1)-O(6) | 148.06(13) | O(8) ^{#2} -Y(2)-O(13) | 151.62(12) |
| Y(1)-O(6) | 2.378(3) | O(1)-Y(1)-O(6) | 101.79(14) | O(15) ^{#2} -Y(2)-O(13) | 81.10(11) |
| Y(1)-OW1 | 2.391(3) | O(7) ^{#2} -Y(1)-O(6) | 127.89(12) | O(5)-Y(2)-O(13) | 101.01(11) |
| Y(1)-O(9) | 2.484(3) | O(10)-Y(1)-O(6) | 84.88(12) | O(2)-Y(2)-O(11) ^{#3} | 106.93(14) |
| Y(1)-O(5) | 2.549(3) | O(16) ^{#1} -Y(1)-OW1 | 84.18(13) | O(8)#2-Y(2)-O(11) ^{#3} | 79.11(13) |

Table S1. Selected bonds lengths (Å) and angles (°) for compounds 1-6

| Y(2)-O(2) | 2.286(3) | O(1)-Y(1)-OW1 | 158.80(12) | O(15)#2-Y(2)-O(11) ^{#3} | 84.33(13) |
|--------------------------|------------|-----------------------------------|------------|--|------------|
| Y(2)-O(8) ^{#2} | 2.300(3) | O(7) ^{#2} -Y(1)-OW1 | 80.12(12) | O(5)-Y(2)-O(11) ^{#3} | 158.28(12) |
| Y(2)-O(15) ^{#2} | 2.318(3) | O(10)-Y(1)-OW1 | 127.21(12) | O(13)-Y(2)-O(11) ^{#3} | 84.01(13) |
| Y(2)-O(5) | 2.369(3) | O(6)-Y(1)-OW1 | 81.56(13) | O(2)-Y(2)-O(12) ^{#3} | 74.41(12) |
| Y(2)-O(13) | 2.378(3) | O(16) ^{#1} -Y(1)-O(9) | 76.57(12) | O(8) ^{#2} -Y(2)-O(12) ^{#3} | 111.41(12) |
| Y(2)-O(11) ^{#3} | 2.390(3) | O(1)-Y(1)-O(9) | 127.96(12) | $O(15)^{#2}$ -Y(2)-O(12) ^{#3} | 132.96(12) |
| Y(2)-O(12) ^{#3} | 2.424(3) | O(7) ^{#2} -Y(1)-O(9) | 143.81(12) | O(5)-Y(2)-O(12) ^{#3} | 148.07(11) |
| Y(2)-O(14) | 2.443(3) | O(10)-Y(1)-O(9) | 54.18(11) | O(13)-Y(2)-O(12) ^{#3} | 75.06(12) |
| O(3)-Co(1)-N(1) | 108.61(17) | O(6)-Y(1)-O(9) | 71.98(11) | $O(11)^{\#3}$ -Y(2)-O(12) ^{#3} | 53.65(12) |
| O(3)-Co(1)-N(3) | 109.02(17) | OW1-Y(1)-O(9) | 73.12(11) | O(2)-Y(2)-O(14) | 81.25(12) |
| N(1)-Co(1)-N(3) | 116.39(18) | O(16) ^{#1} -Y(1)-O(5) | 153.18(12) | O(8) ^{#2} -Y(2)-O(14) | 153.98(12) |
| O(3)-Co(1)-N(2) | 91.60(18) | O(1)-Y(1)-O(5) | 81.64(12) | O(15) ^{#2} -Y(2)-O(14) | 120.87(11) |
| N(1)-Co(1)-N(2) | 108.58(17) | O(7) ^{#2} -Y(1)-O(5) | 77.35(11) | O(5)-Y(2)-O(14) | 77.85(11) |
| N(3)-Co(1)-N(2) | 119.47(18) | O(10)-Y(1)-O(5) | 124.68(12) | O(13)-Y(2)-O(14) | 53.77(11) |
| O(3)-Co(1)-N(4) | 167.67(18) | O(6)-Y(1)-O(5) | 52.48(10) | O(11) ^{#3} -Y(2)-O(14) | 120.69(12) |
| N(1)-Co(1)-N(4) | 77.40(17) | OW1-Y(1)-O(5) | 84.14(11) | O(12) ^{#3} -Y(2)-O(14) | 74.53(11) |
| Compound 2 ^b | | | | | |
| Zn-O(3) | 1.953(3) | N(3)-Zn-N(4) | 76.30(13) | O(9)-Y(1)-O(5) | 121.94(7) |
| Zn-N(1) | 2.057(3) | N(2)-Zn-N(4) | 75.90(13) | O(2)-Y(2)-O(8) ^{#2} | 76.32(10) |
| Zn-N(3) | 2.062(3) | O(16) ^{#1} -Y(1)-O(1) | 100.92(11) | O(2)-Y(2)-O(15) ^{#2} | 145.51(9) |
| Zn-N(2) | 2.092(3) | $O(16)^{\#1}$ -Y(1)-O(7) $^{\#2}$ | 76.84(9) | $O(8)^{#2}$ -Y(2)-O(15) ^{#2} | 74.24(9) |
| Zn-N(4) | 2.291(3) | O(1)-Y(1)-O(7) ^{#2} | 81.73(10) | O(2)-Y(2)-O(5) | 86.09(9) |
| Y(1)-O(16) ^{#1} | 2.226(2) | O(16) ^{#1} -Y(1)-O(10) | 80.98(9) | O(8) ^{#2} -Y(2)-O(5) | 87.83(8) |
| Y(1)-O(1) | 2.243(3) | O(1)-Y(1)-O(10) | 74.52(9) | O(15) ^{#2} -Y(2)-O(5) | 75.29(9) |
| Y(1)-O(7) ^{#2} | 2.303(2) | O(7) ^{#2} -Y(1)-O(10) | 143.59(10) | O(2)-Y(2)-O(13) | 131.47(9) |
| Y(1)-O(10) | 2.326(3) | O(16) ^{#1} -Y(1)-O(6) | 148.35(10) | O(8) ^{#2} -Y(2)-O(13) | 150.91(9) |
| Y(1)-O(6) | 2.387(2) | O(1)-Y(1)-O(6) | 101.90(10) | O(15) ^{#2} -Y(2)-O(13) | 81.21(8) |
| Y(1)-OW1 | 2.394(3) | O(7) ^{#2} -Y(1)-O(6) | 128.05(9) | O(5)-Y(2)-O(13) | 100.94(8) |
| Y(1)-O(9) | 2.491(2) | O(10)-Y(1)-O(6) | 84.29(9) | O(2)-Y(2)-O(11) ^{#3} | 107.34(11) |
| Y(1)-O(5) | 2.544(2) | O(16) ^{#1} -Y(1)-OW1 | 83.74(10) | O(8) ^{#2} -Y(2)-O(11) ^{#3} | 79.13(9) |

| Y(2)-O(2) | 2.295(3) | O(1)-Y(1)-OW1 | 159.27(9) | $O(15)^{#2}-Y(2)-O(11)^{#3}$ | 84.34(10) |
|---------------------------|------------|------------------------------------|-----------|--|-----------|
| Y(2)-O(8) ^{#2} | 2.295(2) | O(7) ^{#2} -Y(1)-OW1 | 79.69(10) | O(5)-Y(2)-O(11) ^{#3} | 158.21(9) |
| Y(2)-O(15) ^{#2} | 2.323(3) | O(10)-Y(1)-OW1 | 126.20(9) | O(13)-Y(2)-O(11) ^{#3} | 83.21(10) |
| Y(2)-O(5) | 2.375(2) | O(6)-Y(1)-OW1 | 82.64(10) | O(2)-Y(2)-O(12) ^{#3} | 74.44(9) |
| Y(2)-O(13) | 2.377(2) | O(16) ^{#1} -Y(1)-O(9) | 76.86(9) | O(8) ^{#2} -Y(2)-O(12) ^{#3} | 111.17(9) |
| Y(2)-O(11) ^{#3} | 2.403(3) | O(1)-Y(1)-O(9) | 128.61(9) | $O(15)^{#2}$ -Y(2)-O(12) ^{#3} | 133.52(9) |
| Y(2)-O(12) ^{#3} | 2.418(3) | O(7) ^{#2} -Y(1)-O(9) | 143.08(9) | O(5)-Y(2)-O(12) ^{#3} | 147.97(9) |
| Y(2)-O(14) | 2.448(2) | O(10)-Y(1)-O(9) | 54.24(9) | O(13)-Y(2)-O(12) ^{#3} | 75.21(9) |
| O(3)-Zn-N(1) | 108.36(13) | O(6)-Y(1)-O(9) | 71.80(8) | $O(11)^{#3}$ -Y(2)-O(12) ^{#3} | 53.81(9) |
| O(3)-Zn-N(3) | 109.85(14) | OW1-Y(1)-O(9) | 72.10(9) | O(2)-Y(2)-O(14) | 82.01(9) |
| N(1)-Zn-N(3) | 116.67(13) | O(16) ^{#1} -Y(1)-O(5) | 153.18(9) | O(8) ^{#2} -Y(2)-O(14) | 154.72(9) |
| O(3)-Zn-N(2) | 91.07(13) | O(1)-Y(1)-O(5) | 82.35(9) | O(15) ^{#2} -Y(2)-O(14) | 120.68(9) |
| N(1)-Zn-N(2) | 108.81(13) | O(7) ^{#2} -Y(1)-O(5) | 77.34(8) | O(5)-Y(2)-O(14) | 77.76(8) |
| N(3)-Zn-N(2) | 118.79(14) | O(10)-Y(1)-O(5) | 125.01(8) | O(13)-Y(2)-O(14) | 53.77(8) |
| O(3)-Zn-N(4) | 166.91(13) | O(6)-Y(1)-O(5) | 52.55(7) | O(11) ^{#3} -Y(2)-O(14) | 120.30(9) |
| N(1)-Zn-N(4) | 77.60(13) | OW1-Y(1)-O(5) | 84.67(8) | O(12) ^{#3} -Y(2)-O(14) | 74.58(9) |
| Compound 3 ^c | | | | | |
| Co(1)-O(3) | 1.955(7) | N(3)-Co(1)-N(4) | 76.0(4) | O(9)-Er(1)-O(5) | 122.1(2) |
| Co(1)-N(1) | 2.058(10) | N(2)-Co(1)-N(4) | 76.5(4) | O(2)-Er(2)-O(8) ^{#2} | 75.9(3) |
| Co(1)-N(3) | 2.072(10) | O(16) ^{#1} -Er(1)-O(1) | 101.1(3) | O(2)-Er(2)-O(15) ^{#2} | 146.0(3) |
| Co(1)-N(2) | 2.091(10) | $O(16)^{\#1}$ -Er(1)-O(7) $^{\#2}$ | 76.7(3) | O(8)#2-Er(2)-O(15) ^{#2} | 74.8(3) |
| Co(1)-N(4) | 2.235(10) | O(1)-Er(1)-O(7) ^{#2} | 82.1(3) | O(2)-Er(2)-O(5) | 85.8(3) |
| Er(1)-O(16) ^{#1} | 2.212(7) | O(16) ^{#1} -Er(1)-O(10) | 80.8(3) | O(8) ^{#2} -Er(2)-O(5) | 87.6(2) |
| Er(1)-O(1) | 2.233(7) | O(1)-Er(1)-O(10) | 73.9(3) | O(15) ^{#2} -Er(2)-O(5) | 76.1(3) |
| ${\rm Er(1)-O(7)}^{\#2}$ | 2.287(8) | O(7) ^{#2} -Er(1)-O(10) | 143.1(3) | O(2)-Er(2)-O(13) | 131.5(3) |
| Er(1)-O(10) | 2.339(8) | O(16) ^{#1} -Er(1)-OW1 | 83.7(3) | O(8) ^{#2} -Er(2)-O(13) | 151.4(3) |
| Er(1)-OW1 | 2.377(7) | O(1)-Er(1)-OW1 | 159.7(3) | O(15) ^{#2} -Er(2)-O(13) | 80.8(2) |
| Er(1)-O(6) | 2.381(7) | O(7) ^{#2} -Er(1)-OW1 | 79.8(3) | O(5)-Er(2)-O(13) | 100.9(2) |
| Er(1)-O(9) | 2.478(7) | O(10)-Er(1)-OW1 | 126.4(3) | O(2)-Er(2)-O(11) ^{#3} | 107.4(3) |
| Er(1)-O(5) | 2.536(7) | O(16) ^{#1} -Er(1)-O(6) | 148.0(3) | $O(8)^{#2}$ -Er(2)- $O(11)^{#3}$ | 79.6(3) |

| Er(2)-O(2) | 2.290(8) | O(1)-Er(1)-O(6) | 101.9(3) | $O(15)^{#2}$ -Er(2)- $O(11)^{#3}$ | 83.8(3) |
|--------------------------------|----------|------------------------------------|------------|------------------------------------|------------|
| ${\rm Er}(2)-{\rm O}(8)^{\#2}$ | 2.291(7) | O(7) ^{#2} -Er(1)-O(6) | 128.4(3) | O(5)-Er(2)-O(11) ^{#3} | 158.5(3) |
| Er(2)-O(15) ^{#2} | 2.328(8) | O(10)-Er(1)-O(6) | 84.5(3) | O(13)-Er(2)-O(11) ^{#3} | 83.2(3) |
| Er(2)-O(5) | 2.369(7) | OW1-Er(1)-O(6) | 82.5(3) | O(2)-Er(2)-O(12) ^{#3} | 74.1(3) |
| Er(2)-O(13) | 2.374(7) | O(16) ^{#1} -Er(1)-O(9) | 76.7(3) | $O(8)^{#2}$ -Er(2)- $O(12)^{#3}$ | 111.0(3) |
| Er(2)-O(11) ^{#3} | 2.395(8) | O(1)-Er(1)-O(9) | 128.0(3) | $O(15)^{#2}$ -Er(2)- $O(12)^{#3}$ | 133.2(3) |
| $Er(2)-O(12)^{\#3}$ | 2.428(8) | O(7) ^{#2} -Er(1)-O(9) | 143.1(3) | O(5)-Er(2)-O(12) ^{#3} | 147.5(3) |
| Er(2)-O(14) | 2.438(7) | O(10)-Er(1)-O(9) | 54.3(2) | O(13)-Er(2)-O(12) ^{#3} | 75.7(3) |
| O(3)-Co(1)-N(1) | 108.6(4) | OW1-Er(1)-O(9) | 72.2(3) | $O(11)^{#3}$ -Er(2)- $O(12)^{#3}$ | 53.9(3) |
| O(3)-Co(1)-N(3) | 109.0(4) | O(6)-Er(1)-O(9) | 71.7(2) | O(2)-Er(2)-O(14) | 81.7(3) |
| N(1)-Co(1)-N(3) | 116.7(4) | $O(16)^{\#1}$ -Er(1)-O(5) | 153.4(3) | O(8) ^{#2} -Er(2)-O(14) | 153.9(3) |
| O(3)-Co(1)-N(2) | 91.9(4) | O(1)-Er(1)-O(5) | 82.2(3) | O(15) ^{#2} -Er(2)-O(14) | 120.9(3) |
| N(1)-Co(1)-N(2) | 109.4(4) | O(7) ^{#2} -Er(1)-O(5) | 77.7(2) | O(5)-Er(2)-O(14) | 77.4(2) |
| N(3)-Co(1)-N(2) | 118.1(4) | O(10)-Er(1)-O(5) | 124.8(3) | O(13)-Er(2)-O(14) | 54.1(2) |
| O(3)-Co(1)-N(4) | 168.3(4) | OW1-Er(1)-O(5) | 84.9(2) | O(11) ^{#3} -Er(2)-O(14) | 120.4(3) |
| N(1)-Co(1)-N(4) | 77.2(4) | O(6)-Er(1)-O(5) | 52.7(2) | O(12) ^{#3} -Er(2)-O(14) | 74.6(3) |
| Compound 4 ^d | | | | | |
| Zn(1)-O(3) | 1.947(3) | N(3)-Zn(1)-N(4) | 76.32(15) | O(9)-Er(1)-O(5) | 122.59(9) |
| Zn(1)-N(1) | 2.060(4) | N(2)-Zn(1)-N(4) | 75.72(16) | O(2)-Er(2)-O(8) ^{#2} | 76.43(12) |
| Zn(1)-N(3) | 2.061(4) | O(16) ^{#1} -Er(1)-O(1) | 101.49(13) | O(2)-Er(2)-O(15) ^{#2} | 146.48(11) |
| Zn(1)-N(2) | 2.099(4) | $O(16)^{\#1}$ -Er(1)-O(7) $^{\#2}$ | 76.91(12) | $O(8)^{\#2}$ -Er(2)- $O(15)^{\#2}$ | 74.96(11) |
| Zn(1)-N(4) | 2.287(4) | O(1)-Er(1)-O(7) ^{#2} | 81.88(13) | O(2)-Er(2)-O(13) | 130.52(11) |
| Er(1)-O(16) ^{#1} | 2.211(3) | O(16) ^{#1} -Er(1)-O(10) | 81.19(12) | O(8) ^{#2} -Er(2)-O(13) | 151.87(11) |
| Er(1)-O(1) | 2.229(3) | O(1)-Er(1)-O(10) | 73.73(11) | O(15) ^{#2} -Er(2)-O(13) | 81.10(10) |
| $Er(1)-O(7)^{#2}$ | 2.292(3) | O(7) ^{#2} -Er(1)-O(10) | 143.04(12) | O(2)-Er(2)-O(5) | 86.05(11) |
| Er(1)-O(10) | 2.318(3) | O(16) ^{#1} -Er(1)-O(6) | 148.09(12) | O(8) ^{#2} -Er(2)-O(5) | 87.54(10) |
| Er(1)-O(6) | 2.368(3) | O(1)-Er(1)-O(6) | 101.92(13) | O(15) ^{#2} -Er(2)-O(5) | 75.67(10) |
| Er(1)-OW1 | 2.376(3) | O(7) ^{#2} -Er(1)-O(6) | 127.80(11) | O(13)-Er(2)-O(5) | 100.77(10) |
| Er(1)-O(9) | 2.482(3) | O(10)-Er(1)-O(6) | 84.88(11) | O(2)-Er(2)-O(11) ^{#3} | 107.80(13) |
| Er(1)-O(5) | 2.539(3) | O(16) ^{#1} -Er(1)-OW1 | 84.34(12) | $O(8)^{#2}$ -Er(2)- $O(11)^{#3}$ | 79.46(12) |

| Er(2)-O(2) | 2.282(3) | O(1)-Er(1)-OW1 | 159.26(11) | $O(15)^{#2}$ -Er(2)- $O(11)^{#3}$ | 83.73(12) |
|--------------------------------|------------|----------------------------------|------------|-----------------------------------|------------|
| ${\rm Er}(2)-{\rm O}(8)^{\#2}$ | 2.285(3) | O(7) ^{#2} -Er(1)-OW1 | 80.10(12) | O(13)-Er(2)-O(11) ^{#3} | 83.49(12) |
| Er(2)-O(15) ^{#2} | 2.314(3) | O(10)-Er(1)-OW1 | 127.00(11) | O(5)-Er(2)-O(11) ^{#3} | 157.94(11) |
| Er(2)-O(13) | 2.365(3) | O(6)-Er(1)-OW1 | 81.40(11) | $O(2)$ -Er(2)- $O(12)^{\#3}$ | 74.05(12) |
| Er(2)-O(5) | 2.367(3) | O(16) ^{#1} -Er(1)-O(9) | 76.63(12) | $O(8)^{#2}$ -Er(2)- $O(12)^{#3}$ | 111.00(12) |
| Er(2)-O(11) ^{#3} | 2.377(3) | O(1)-Er(1)-O(9) | 127.75(11) | $O(15)^{#2}$ -Er(2)- $O(12)^{#3}$ | 133.15(11) |
| Er(2)-O(12) ^{#3} | 2.416(3) | O(7) ^{#2} -Er(1)-O(9) | 143.63(11) | O(13)-Er(2)-O(12) ^{#3} | 75.39(12) |
| Er(2)-O(14) | 2.447(3) | O(10)-Er(1)-O(9) | 54.21(10) | O(5)-Er(2)-O(12) ^{#3} | 148.01(10) |
| O(3)-Zn(1)-N(1) | 108.68(17) | O(6)-Er(1)-O(9) | 71.93(10) | $O(11)^{#3}$ -Er(2)- $O(12)^{#3}$ | 54.05(11) |
| O(3)-Zn(1)-N(3) | 109.45(16) | OW1-Er(1)-O(9) | 72.88(10) | O(2)-Er(2)-O(14) | 80.88(11) |
| N(1)-Zn(1)-N(3) | 116.79(16) | O(16) ^{#1} -Er(1)-O(5) | 153.22(11) | O(8) ^{#2} -Er(2)-O(14) | 153.70(11) |
| O(3)-Zn(1)-N(2) | 91.16(16) | O(1)-Er(1)-O(5) | 81.69(11) | O(15) ^{#2} -Er(2)-O(14) | 120.98(10) |
| N(1)-Zn(1)-N(2) | 107.81(16) | O(7) ^{#2} -Er(1)-O(5) | 77.26(10) | O(13)-Er(2)-O(14) | 53.85(9) |
| N(3)-Zn(1)-N(2) | 119.65(17) | O(10)-Er(1)-O(5) | 124.61(10) | O(5)-Er(2)-O(14) | 77.71(10) |
| O(3)-Zn(1)-N(4) | 166.74(16) | O(6)-Er(1)-O(5) | 52.61(9) | O(11) ^{#3} -Er(2)-O(14) | 120.63(11) |
| N(1)-Zn(1)-N(4) | 77.79(16) | OW1-Er(1)-O(5) | 84.41(10) | O(12) ^{#3} -Er(2)-O(14) | 74.63(11) |
| Compound 5 ^e | | | | | |
| Co(1)-O(3) | 1.959(13) | O(1)-Sm(1)-O(10) | 71.3(5) | O(15) ^{#2} -Sm(2)-O(2') | 131.9(6) |
| Co(1)-N(3) | 2.046(7) | O(16) ^{#1} -Sm(1)-O(10) | 79.7(4) | O(8) ^{#2} -Sm(2)-O(5) | 94.4(4) |
| Co(1)-O(4') | 2.05(3) | O(7) ^{#2} -Sm(1)-O(10) | 145.4(4) | O(15) ^{#2} -Sm(2)-O(5) | 75.4(4) |
| Co(1)-N(1) | 2.052(6) | O(1)-Sm(1)-OW1 | 161.6(5) | O(2')-Sm(2)-O(5) | 62.4(6) |
| Co(1)-N(2) | 2.062(8) | O(16) ^{#1} -Sm(1)-OW1 | 86.3(4) | O(8) ^{#2} -Sm(2)-O(13) | 151.6(4) |
| Co(1)-N(4) | 2.217(11) | O(7) ^{#2} -Sm(1)-OW1 | 79.2(3) | O(15) ^{#2} -Sm(2)-O(13) | 81.5(3) |
| Sm(1)-O(1) | 2.200(14) | O(10)-Sm(1)-OW1 | 126.5(4) | O(2')-Sm(2)-O(13) | 125.2(6) |
| Sm(1)-O(16) ^{#1} | 2.277(10) | O(1)-Sm(1)-O(6) | 106.6(6) | O(5)-Sm(2)-O(13) | 99.1(3) |
| $Sm(1)-O(7)^{\#2}$ | 2.385(10) | O(16) ^{#1} -Sm(1)-O(6) | 148.5(4) | O(8) ^{#2} -Sm(2)-O(2) | 71.7(6) |
| Sm(1)-O(10) | 2.419(9) | O(7) ^{#2} -Sm(1)-O(6) | 126.2(3) | O(15) ^{#2} -Sm(2)-O(2) | 145.8(6) |
| Sm(1)-OW1 | 2.425(8) | O(10)-Sm(1)-O(6) | 83.9(3) | O(2')-Sm(2)-O(2) | 30.1(6) |
| Sm(1)-O(6) | 2.480(9) | OW1-Sm(1)-O(6) | 82.1(3) | O(5)-Sm(2)-O(2) | 91.4(5) |
| Sm(1)-O(9) | 2.514(9) | O(1)-Sm(1)-O(9) | 124.5(4) | O(13)-Sm(2)-O(2) | 132.3(5) |

| Sm(1)-O(5) | 2.607(9) | O(16) ^{#1} -Sm(1)-O(9) | 77.1(4) | $O(8)^{\#2}$ -Sm(2)-O(12) ^{#3} 103.3(4) |
|--------------------------------|-----------|---|----------|---|
| Sm(1)-O(2') | 2.82(2) | O(7) ^{#2} -Sm(1)-O(9) | 144.8(3) | $O(15)^{\#2}$ -Sm(2)-O(12) ^{#3} 132.3(4) |
| Sm(1)-O(1') | 2.84(3) | O(10)-Sm(1)-O(9) | 53.1(3) | O(2')-Sm(2)-O(12) ^{#3} 94.8(6) |
| Sm(2)-O(8) ^{#2} | 2.324(11) | OW1-Sm(1)-O(9) | 73.4(3) | $O(5)-Sm(2)-O(12)^{\#3}$ 149.4(3) |
| Sm(2)-O(15) ^{#2} | 2.355(10) | O(6)-Sm(1)-O(9) | 71.6(3) | O(13)-Sm(2)-O(12) ^{#3} 76.8(4) |
| Sm(2)-O(2') | 2.36(2) | O(1)-Sm(1)-O(5) | 92.0(5) | $O(2)-Sm(2)-O(12)^{\#3}$ 71.2(5) |
| Sm(2)-O(5) | 2.412(9) | O(16) ^{#1} -Sm(1)-O(5) | 154.6(3) | $O(8)^{\#2}-Sm(2)-O(11')^{\#3}$ 67.3(6) |
| Sm(2)-O(13) | 2.434(10) | O(7) ^{#2} -Sm(1)-O(5) | 76.6(3) | $O(15)^{#2}$ -Sm(2)-O(11') ^{#3} 89.7(5) |
| Sm(2)-O(2) | 2.441(17) | O(10)-Sm(1)-O(5) | 125.4(4) | O(2')-Sm(2)-O(11') ^{#3} 122.6(7) |
| Sm(2)-O(12) ^{#3} | 2.476(10) | OW1-Sm(1)-O(5) | 81.0(3) | O(5)-Sm(2)-O(11') ^{#3} 158.7(4) |
| Sm(2)-O(11') ^{#3} | 2.50(2) | O(6)-Sm(1)-O(5) | 50.8(3) | O(13)-Sm(2)-O(11') ^{#3} 93.5(5) |
| Sm(2)-O(11) ^{#3} | 2.518(17) | O(9)-Sm(1)-O(5) | 119.4(3) | $O(2)-Sm(2)-O(11')^{\#3}$ 92.7(7) |
| Sm(2)-O(14) | 2.558(9) | O(1)-Sm(1)-O(2') | 38.0(6) | $O(12)^{\#3}$ -Sm(2)- $O(11')^{\#3}$ 50.6(5) |
| O(3)-Co(1)-N(3) | 110.6(5) | O(16) ^{#1} -Sm(1)-O(2') | 127.0(6) | $O(8)^{\#2}-Sm(2)-O(11)^{\#3}$ 83.8(5) |
| O(3)-Co(1)-O(4') | 35.3(9) | O(7) ^{#2} -Sm(1)-O(2') | 75.3(5) | O(15)#2-Sm(2)-O(11)#379.2(5) |
| N(3)-Co(1)-O(4') | 95.2(8) | O(10)-Sm(1)-O(2') | 95.8(5) | $O(2')-Sm(2)-O(11)^{\#3}$ 142.0(7) |
| O(3)-Co(1)-N(1) | 110.2(5) | OW1-Sm(1)-O(2') | 132.0(5) | $O(5)-Sm(2)-O(11)^{\#3}$ 154.3(5) |
| N(3)-Co(1)-N(1) | 116.8(3) | O(6)-Sm(1)-O(2') | 81.2(5) | O(13)-Sm(2)-O(11) ^{#3} 73.3(5) |
| O(4')-Co(1)-N(1) | 91.6(8) | O(9)-Sm(1)-O(2') | 139.8(5) | $O(2)-Sm(2)-O(11)^{\#3}$ 112.0(7) |
| O(3)-Co(1)-N(2) | 87.8(5) | O(5)-Sm(1)-O(2') | 54.0(5) | $O(12)^{\#3}$ -Sm(2)-O(11) ^{#3} 54.2(5) |
| N(3)-Co(1)-N(2) | 118.1(4) | O(1)-Sm(1)-O(1') | 13.4(8) | $O(11')^{\#3}$ -Sm(2)- $O(11)^{\#3}$ 21.7(5) |
| O(4')-Co(1)-N(2) | 122.8(9) | O(16) ^{#1} -Sm(1)-O(1') | 82.7(7) | O(8) ^{#2} -Sm(2)-O(14) 154.8(4) |
| N(1)-Co(1)-N(2) | 109.4(3) | O(7) ^{#2} -Sm(1)-O(1') | 72.6(6) | O(15) ^{#2} -Sm(2)-O(14) 121.8(3) |
| O(3)-Co(1)-N(4) | 164.5(6) | O(10)-Sm(1)-O(1') | 77.5(6) | O(2')-Sm(2)-O(14) 71.9(6) |
| N(3)-Co(1)-N(4) | 76.4(4) | OW1-Sm(1)-O(1') | 151.2(6) | O(5)-Sm(2)-O(14) 77.7(3) |
| O(4')-Co(1)-N(4) | 160.1(9) | O(6)-Sm(1)-O(1') | 119.7(6) | O(13)-Sm(2)-O(14) 53.4(3) |
| N(1)-Co(1)-N(4) | 76.8(4) | O(9)-Sm(1)-O(1') | 129.0(6) | O(2)-Sm(2)-O(14) 84.5(6) |
| N(2)-Co(1)-N(4) | 76.7(4) | O(5)-Sm(1)-O(1') | 98.1(6) | O(12) ^{#3} -Sm(2)-O(14) 75.8(3) |
| O(1)-Sm(1)-O(16) ^{#1} | 93.4(6) | O(2')-Sm(1)-O(1') | 45.4(7) | O(11') ^{#3} -Sm(2)-O(14) 123.5(5) |
| O(1)-Sm(1)-O(7) ^{#2} | 82.6(5) | O(8) ^{#2} -Sm(2)-O(15) ^{#2} | 77.9(4) | O(11) ^{#3} -Sm(2)-O(14) 113.6(4) |

| $O(16)^{\#1}-Sm(1)-O(7)^{\#1}$ | ² 79.5(4) | $O(8)^{#2}-Sm(2)-O(2')$ | 83.2(6) | | |
|--------------------------------|----------------------|-------------------------|-----------|---|-----------|
| Compound 6 ^f | | | | | |
| Ni(1)-O(1) | 2.00(4) | N(10)-Ni(2)-O(20) | 97.6(16) | O(13)-Y(1)-O(5) | 136.1(12) |
| Ni(1)-N(1) | 2.01(4) | N(10)-Ni(2)-N(12) | 93.2(17) | O(15) ^{#1} -Y(2)-O(16) | 105.7(13) |
| Ni(1)-N(3) | 2.02(4) | O(20)-Ni(2)-N(12) | 101.7(17) | O(15) ^{#1} -Y(2)-O(18) | 154.7(13) |
| Ni(1)-N(5) | 2.02(4) | N(10)-Ni(2)-N(8) | 98.3(17) | O(16)-Y(2)-O(18) | 77.2(13) |
| Ni(1)-N(7) | 2.27(4) | O(20)-Ni(2)-N(8) | 101.0(17) | $O(15)^{\#1}$ -Y(2)-O(8) $^{\#2}$ | 102.3(14) |
| Ni(2)-N(10) | 2.00(4) | N(12)-Ni(2)-N(8) | 152.8(18) | O(16)-Y(2)-O(8) ^{#2} | 151.1(14) |
| Ni(2)-O(20) | 2.01(4) | N(10)-Ni(2)-N(14) | 80.8(16) | O(18)-Y(2)-O(8) ^{#2} | 80.6(14) |
| Ni(2)-N(12) | 2.03(4) | O(20)-Ni(2)-N(14) | 177.6(16) | O(15) ^{#1} -Y(2)-OW10 | 77.2(14) |
| Ni(2)-N(8) | 2.05(4) | N(12)-Ni(2)-N(14) | 80.2(17) | O(16)-Y(2)-OW10 | 68.0(15) |
| Ni(2)-N(14) | 2.25(4) | N(8)-Ni(2)-N(14) | 77.5(16) | O(18)-Y(2)-OW10 | 125.5(14) |
| Y(1)-O(3) | 2.23(4) | O(3)-Y(1)-O(9) | 158.8(12) | O(8) ^{#2} -Y(2)-OW10 | 112.4(15) |
| Y(1)-O(9) | 2.26(3) | O(3)-Y(1)-OW9 | 98.6(14) | O(15) ^{#1} -Y(2)-O(17) | 151.0(13) |
| Y(1)-OW9 | 2.32(4) | O(9)-Y(1)-OW9 | 85.8(14) | O(16)-Y(2)-O(17) | 79.6(13) |
| Y(1)-OW8 | 2.34(3) | O(3)-Y(1)-OW8 | 89.5(13) | O(18)-Y(2)-O(17) | 54.1(12) |
| Y(1)-O(6) | 2.38(3) | O(9)-Y(1)-OW8 | 95.0(12) | O(8) ^{#2} -Y(2)-O(17) | 72.5(14) |
| Y(1)-O(14) | 2.43(3) | OW9-Y(1)-OW8 | 155.5(12) | OW10-Y(2)-O(17) | 78.7(14) |
| Y(1)-O(13) | 2.43(3) | O(3)-Y(1)-O(6) | 75.8(13) | O(15) ^{#1} -Y(2)-O(11) ^{#1} | 81.6(12) |
| Y(1)-O(5) | 2.54(3) | O(9)-Y(1)-O(6) | 125.3(12) | O(16)-Y(2)-O(11) ^{#1} | 121.0(14) |
| Y(2)-O(15) ^{#1} | 2.25(3) | OW9-Y(1)-O(6) | 77.6(13) | O(18)-Y(2)-O(11) ^{#1} | 75.8(12) |
| Y(2)-O(16) | 2.35(4) | OW8-Y(1)-O(6) | 82.1(13) | O(8) ^{#2} -Y(2)-O(11) ^{#1} | 69.9(13) |
| Y(2)-O(18) | 2.39(3) | O(3)-Y(1)-O(14) | 78.1(13) | OW10-Y(2)-O(11) ^{#1} | 158.6(14) |
| Y(2)-O(8) ^{#2} | 2.42(4) | O(9)-Y(1)-O(14) | 83.0(12) | O(17)-Y(2)-O(11) ^{#1} | 120.8(12) |
| Y(2)-OW10 | 2.44(5) | OW9-Y(1)-O(14) | 76.1(12) | O(15) ^{#1} -Y(2)-O(12) ^{#1} | 74.9(13) |
| Y(2)-O(17) | 2.45(3) | OW8-Y(1)-O(14) | 128.3(12) | O(16)-Y(2)-O(12) ^{#1} | 72.6(13) |
| Y(2)-O(11) ^{#1} | 2.47(3) | O(6)-Y(1)-O(14) | 139.3(13) | O(18)-Y(2)-O(12) ^{#1} | 82.3(12) |
| Y(2)-O(12) ^{#1} | 2.47(4) | O(3)-Y(1)-O(13) | 83.2(13) | $O(8)^{\#2}$ -Y(2)-O(12) ^{#1} | 122.4(13) |
| Y(2)-O(7) ^{#2} | 2.56(4) | O(9)-Y(1)-O(13) | 78.0(12) | OW10-Y(2)-O(12) ^{#1} | 122.2(14) |
| O(1)-Ni(1)-N(1) | 100.0(16) | OW9-Y(1)-O(13) | 128.5(12) | O(17)-Y(2)-O(12) ^{#1} | 132.6(12) |

| O(1)-Ni(1)-N(3) | 100.5(16) | OW8-Y(1)-O(13) | 75.2(11) | $O(11)^{\#1}$ -Y(2)-O(12)^{\#1} | 52.6(12) |
|------------------------------------|-------------------------------|--------------------------------------|---------------------------------|--|--------------------------|
| N(1)-Ni(1)-N(3) | 93.4(17) | O(6)-Y(1)-O(13) | 149.1(12) | O(15) ^{#1} -Y(2)-O(7) ^{#2} | 79.7(12) |
| O(1)-Ni(1)-N(5) | 101.9(17) | O(14)-Y(1)-O(13) | 53.7(11) | O(16)-Y(2)-O(7) ^{#2} | 127.6(15) |
| N(1)-Ni(1)-N(5) | 154.9(18) | O(3)-Y(1)-O(5) | 127.3(12) | O(18)-Y(2)-O(7)# ² | 119.1(13) |
| N(3)-Ni(1)-N(5) | 94.7(17) | O(9)-Y(1)-O(5) | 73.7(11) | $O(8)^{#2}$ -Y(2)-O(7) ^{#2} | 51.4(14) |
| O(1)-Ni(1)-N(7) | 178.4(15) | OW9-Y(1)-O(5) | 82.3(12) | OW10-Y(2)-O(7) ^{#2} | 62.6(15) |
| N(1)-Ni(1)-N(7) | 79.1(16) | OW8-Y(1)-O(5) | 74.5(11) | O(17)-Y(2)-O(7) ^{#2} | 75.0(14) |
| N(3)-Ni(1)-N(7) | 80.9(16) | O(6)-Y(1)-O(5) | 52.7(12) | $O(11)^{\#1}$ -Y(2)-O(7) $^{\#2}$ | 111.4(14) |
| N(5)-Ni(1)-N(7) | 78.7(16) | O(14)-Y(1)-O(5) | 149.3(12) | $O(12)^{\#1}$ -Y(2)-O(7) $^{\#2}$ | 151.5(14) |
| ^{<i>a</i>} Symmetry code: | ^{#1} x, y - 1, z; | $y^{\#2} - x + 3, y - 1/2,$ | -z + 1/2; ^{#3} z | x, -y + 3/2, z - 1/2. | ^b Symmetry |
| code: $^{#1}$ x, y – 1, | $z;^{\#2} - x + 3, y$ | y - 1/2, -z + 1/2; ^{#3} z | x, -y + 3/2, z | - 1/2. ^c Symmetry cod | de: ^{#1} x, y – |
| 1, z; $^{\#2}$ – x + 3, y | z = 1/2, -z + 1 | /2; ^{#3} x, $-y + 3/2, z$ | – 1/2. ^{<i>d</i>} Symm | hetry code: $^{\#1}$ x, y – 1, | z; = x + z; = x + z |
| 3, $y - 1/2$, $-z + 1$ | /2; ^{#3} x, $-y + 3$ | 3/2, z – 1/2. ^e Symm | etry code: #1 x | x, y - 1, z; $^{\#2}$ - x + 3, | y − 1/2, −z |

+ 1/2; ^{#3} x, -y + 3/2, z - 1/2. ^fSymmetry code: ^{#1} - x + 1, -y, -z + 1; ^{#2} x, y, z + 1.



Fig. S1 Experimental (top) and simulated (bottom) XRD patterns for compound 1.



Fig. S2 Experimental (top) and simulated (bottom) XRD patterns for compound 2.



Fig. S3 Experimental (top) and simulated (bottom) XRD patterns for compound 3.



Fig. S4 Experimental (top) and simulated (bottom) XRD patterns for compound 4.



Fig. S5 Experimental (top) and simulated (bottom) XRD patterns for compound 5.



Fig. S6 The 2D structure of 1 viewed in the *bc* plane.



Fig. S7 The 1D structure of 1 viewed along the *c* axis.



Fig. S8 The IR spectra of 1.



Fig. S9 TGA curve of 1.



Fig. S10 TGA curve of 2.



Fig. S11 TGA curve of 3.



Fig. S12 TGA curve of 4.



Fig. S13 TGA curve of 5.