# Supporting Information

## Synthesis, structure, characterization and multifunctional properties of a family of rare earth organic frameworks

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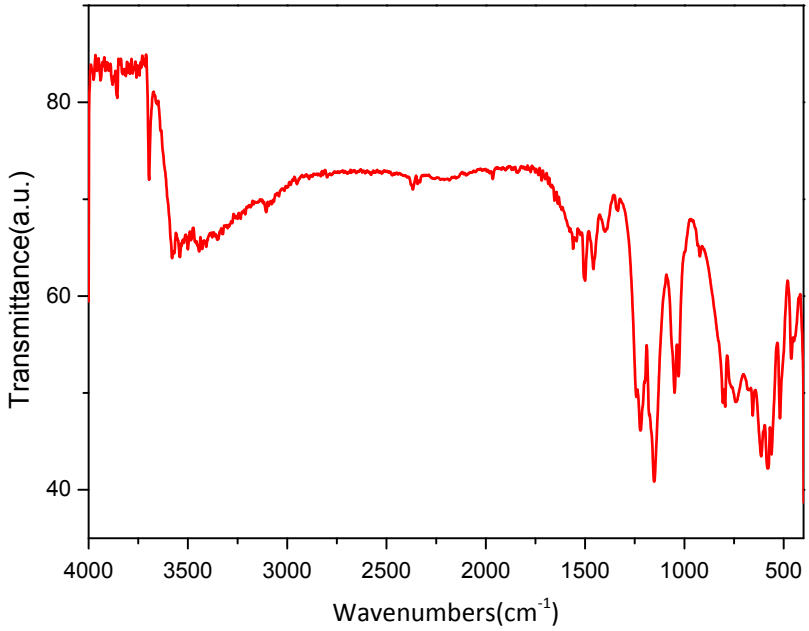


**Fig. S1** IR spectra for compound **1.**

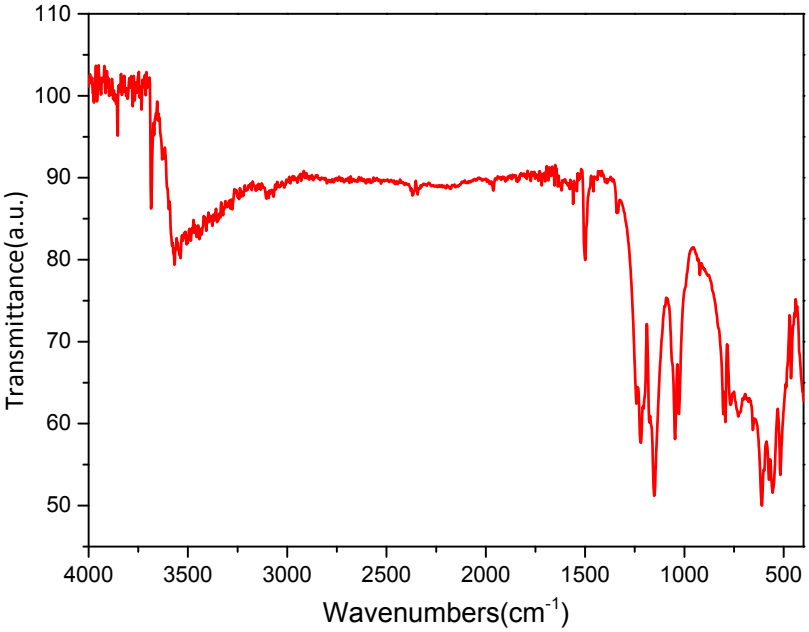


**Fig. S2** IR spectra for compound **2.**

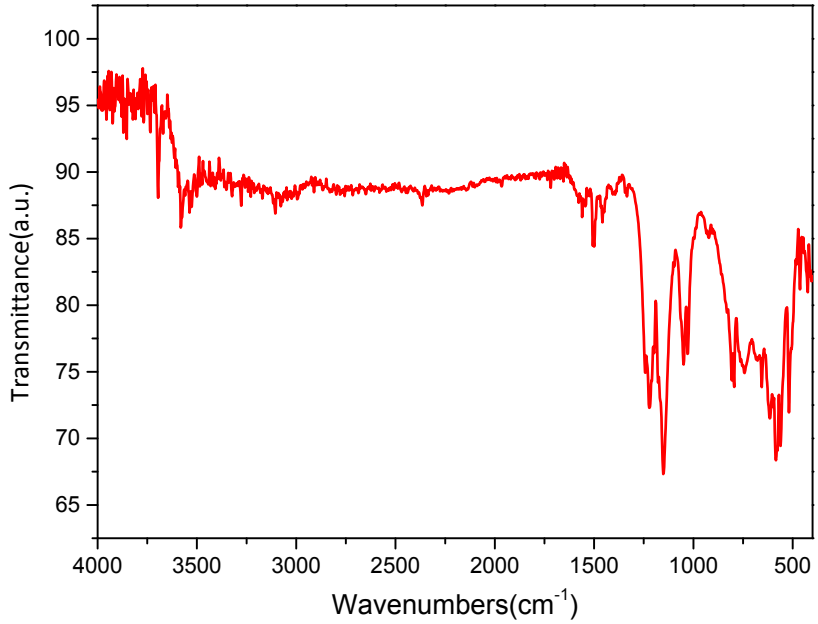


**Fig. S3** IR spectra for compound **3.**

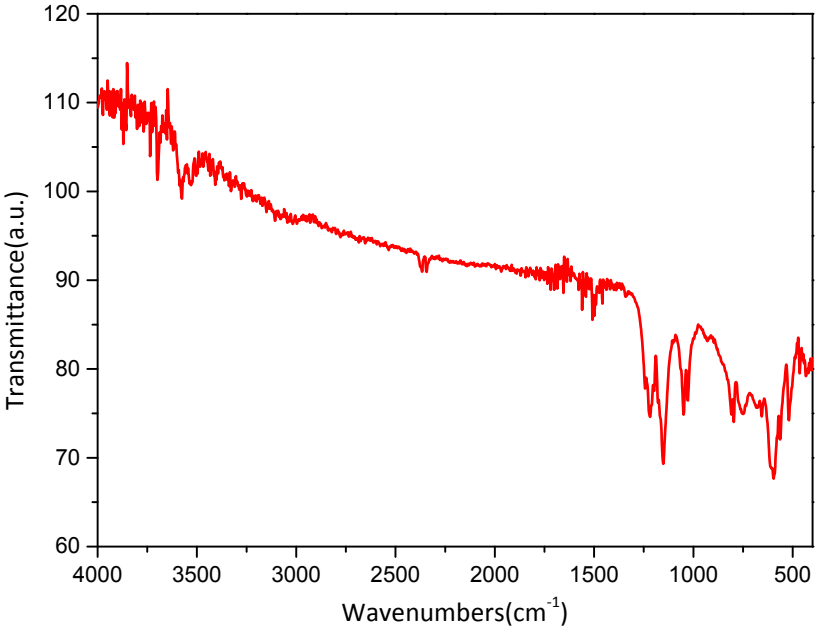


**Fig. S4** IR spectra for compound **4.**

**Table S1** Closest metal-metal distances, selected bond lengths and angles in compound **1**

| Compound 1[a] | | | |
|---|---|---|---|
| Y(1)-O(13) | 2.336(5) | Y(2)-O(8)#3 | 2.374(6) |
| Y(1)-O(11)#1 | 2.345(6) | Y(2)-O(13) | 2.398(5) |
| Y(1)-O(1) | 2.357(6) | Y(2)-O(4) | 2.428(7) |
| Y(1)-O(11) | 2.362(6) | Y(2)-Y(3) | 3.5061(17) |
| Y(1)-O(12) | 2.370(6) | Y(2)-Y(1)#4 | 3.8253(18) |
| Y(1)-O(7) | 2.392(6) | Y(2)-Y(2)#4 | 3.843(2) |
| Y(1)-O(10)#1 | 2.402(5) | Y(3)-O(13) | 2.331(6) |
| Y(1)-O(9)#2 | 2.415(6) | Y(3)-O(9) | 2.361(6) |
| Y(1)-Y(3) | 3.515(2) | Y(3)-O(10) | 2.367(6) |
| Y(1)-Y(2) | 3.5151(16) | Y(3)-O(12) | 2.367(6) |
| Y(1)-Y(3)#2 | 3.721(2) | Y(3)-O(2)#5 | 2.367(6) |
| Y(1)-Y(1)#1 | 3.7997(19) | Y(3)-O(11) | 2.403(6) |
| Y(2)-O(8) | 2.301(6) | Y(3)-O(10)#6 | 2.409(6) |
| Y(2)-O(9)#3 | 2.315(6) | Y(3)-O(8) | 2.464(6) |
| Y(2)-O(7) | 2.320(6) | Y(3)-Y(1)#5 | 3.721(2) |
| Y(2)-O(12) | 2.347(6) | Y(3)-Y(1)#1 | 3.8480(16) |
| Y(2)-O(7)#4 | 2.352(5) | | |
| O(13)-Y(1)-O(11)#1 | 131.6(2) | O(7)#4-Y(2)-O(8)#3 | 75.4(2) |
| O(13)-Y(1)-O(1) | 73.9(2) | O(8)-Y(2)-O(13) | 70.94(19) |
| O(11)#1-Y(1)-O(1) | 138.7(2) | O(9)#3-Y(2)-O(13) | 151.35(19) |
| O(13)-Y(1)-O(11) | 71.0(2) | O(7)-Y(2)-O(13) | 69.45(19) |
| O(11)#1-Y(1)-O(11) | 72.4(2) | O(12)-Y(2)-O(13) | 60.98(19) |
| O(1)-Y(1)-O(11) | 93.3(2) | O(7)#4-Y(2)-O(13) | 129.68(18) |
| O(13)-Y(1)-O(12) | 61.56(19) | O(8)#3-Y(2)-O(13) | 129.0(2) |
| O(11)#1-Y(1)-O(12) | 80.99(19) | O(8)-Y(2)-O(4) | 89.9(2) |
| O(1)-Y(1)-O(12) | 135.02(19) | O(9)#3-Y(2)-O(4) | 77.8(2) |
| O(11)-Y(1)-O(12) | 78.4(2) | O(7)-Y(2)-O(4) | 79.3(2) |
| O(13)-Y(1)-O(7) | 69.30(19) | O(12)-Y(2)-O(4) | 134.4(2) |
| O(11)#1-Y(1)-O(7) | 133.82(19) | O(7)#4-Y(2)-O(4) | 124.1(2) |
| O(1)-Y(1)-O(7) | 81.6(2) | O(8)#3-Y(2)-O(4) | 134.2(2) |
| O(11)-Y(1)-O(7) | 139.85(19) | O(13)-Y(2)-O(4) | 73.9(2) |
| O(12)-Y(1)-O(7) | 77.7(2) | O(13)-Y(3)-O(9) | 135.79(19) |
| O(13)-Y(1)-O(10)#1 | 142.56(19) | O(13)-Y(3)-O(10) | 131.90(19) |
| O(11)#1-Y(1)-O(10)#1 | 72.2(2) | O(9)-Y(3)-O(10) | 76.15(19) |
| O(1)-Y(1)-O(10)#1 | 71.50(19) | O(13)-Y(3)-O(12) | 61.7(2) |
| O(11)-Y(1)-O(10)#1 | 97.11(19) | O(9)-Y(3)-O(12) | 98.3(2) |
| O(12)-Y(1)-O(10)#1 | 152.88(19) | O(10)-Y(3)-O(12) | 82.08(19) |
| O(7)-Y(1)-O(10)#1 | 118.28(19) | O(13)-Y(3)-O(2)#5 | 73.7(2) |
| O(13)-Y(1)-O(9)#2 | 137.17(19) | O(9)-Y(3)-O(2)#5 | 106.7(2) |
| O(11)#1-Y(1)-O(9)#2 | 75.4(2) | O(10)-Y(3)-O(2)#5 | 140.7(2) |
| O(1)-Y(1)-O(9)#2 | 108.7(2) | O(12)-Y(3)-O(2)#5 | 134.0(2) |

| | | | |
|---|---|---|---|
| O(11)-Y(1)-O(9)#2 | 147.5(2) | O(13)-Y(3)-O(11) | 70.4(2) |
| O(12)-Y(1)-O(9)#2 | 100.38(19) | O(9)-Y(3)-O(11) | 148.0(2) |
| O(7)-Y(1)-O(9)#2 | 68.93(19) | O(10)-Y(3)-O(11) | 71.8(2) |
| O(10)#1-Y(1)-O(9)#2 | 69.12(18) | O(12)-Y(3)-O(11) | 77.64(19) |
| O(8)-Y(2)-O(9)#3 | 104.90(19) | O(2)#5-Y(3)-O(11) | 98.0(2) |
| O(8)-Y(2)-O(7) | 140.4(2) | O(13)-Y(3)-O(10)#6 | 143.16(19) |
| O(9)#3-Y(2)-O(7) | 109.7(2) | O(9)-Y(3)-O(10)#6 | 69.89(19) |
| O(8)-Y(2)-O(12) | 81.49(19) | O(10)-Y(3)-O(10)#6 | 71.5(2) |
| O(9)#3-Y(2)-O(12) | 147.61(19) | O(12)-Y(3)-O(10)#6 | 152.9(2) |
| O(7)-Y(2)-O(12) | 79.6(2) | O(2)#5-Y(3)-O(10)#6 | 73.0(2) |
| O(8)-Y(2)-O(7)#4 | 142.3(2) | O(11)-Y(3)-O(10)#6 | 99.26(19) |
| O(9)#3-Y(2)-O(7)#4 | 71.31(19) | O(13)-Y(3)-O(8) | 69.28(19) |
| O(7)-Y(2)-O(7)#4 | 69.3(2) | O(9)-Y(3)-O(8) | 68.0(2) |
| O(12)-Y(2)-O(7)#4 | 84.24(19) | O(10)-Y(3)-O(8) | 135.31(19) |
| O(8)-Y(2)-O(8)#3 | 68.4(2) | O(12)-Y(3)-O(8) | 77.77(18) |
| O(9)#3-Y(2)-O(8)#3 | 70.3(2) | O(2)#5-Y(3)-O(8) | 76.9(2) |
| O(7)-Y(2)-O(8)#3 | 141.99(19) | O(11)-Y(3)-O(8) | 139.1(2) |
| O(12)-Y(2)-O(8)#3 | 83.4(2) | O(10)#6-Y(3)-O(8) | 117.06(18) |

[a]Symmetry codes: (#1) -x-2,-y+2,-z+1; (#2) -x-3,-y+2,-z+1; (#3) -x-2,-y+1,-z+1; (#4) x+1,y,z; (#5) x-1,y,z; (#6) -x-3,-y+1,-z+1; (#7) -x-3,-y+2,-z+2; (#8) -x-2,-y+1,-z+2

**Table S2** Closest metal-metal distances, selected bond lengths and angles in compound **2**

| **Compound 2[b]** | | | |
|---|---|---|---|
| Gd(1)-O(11)#1 | 2.356(7) | Gd(2)-O(12) | 2.410(7) |
| Gd(1)-O(11) | 2.356(8) | Gd(2)-O(8)#3 | 2.429(7) |
| Gd(1)-O(12) | 2.391(7) | Gd(2)-O(4) | 2.453(8) |
| Gd(1)-O(13) | 2.414(7) | Gd(2)-Gd(3) | 3.580(3) |
| Gd(1)-O(1) | 2.416(7) | Gd(2)-Gd(1)#4 | 3.900(3) |
| Gd(1)-O(9)#2 | 2.434(7) | Gd(2)-Gd(3)#3 | 3.936(3) |
| Gd(1)-O(7) | 2.454(8) | Gd(3)-O(12) | 2.367(9) |
| Gd(1)-O(10)#1 | 2.453(7) | Gd(3)-O(13) | 2.388(7) |
| Gd(1)-Gd(2) | 3.583(3) | Gd(3)-O(9) | 2.390(7) |
| Gd(1)-Gd(3) | 3.594(3) | Gd(3)-O(10) | 2.393(7) |
| Gd(1)-Gd(3)#2 | 3.779(3) | Gd(3)-O(2)#5 | 2.419(7) |
| Gd(1)-Gd(1)#1 | 3.878(3) | Gd(3)-O(10)#6 | 2.451(8) |
| Gd(2)-O(7) | 2.331(8) | Gd(3)-O(8) | 2.472(8) |
| Gd(2)-O(8) | 2.364(8) | Gd(3)-O(11) | 2.494(7) |
| Gd(2)-O(9)#3 | 2.368(7) | Gd(3)-Gd(1)#5 | 3.779(3) |
| Gd(2)-O(13) | 2.380(7) | Gd(3)-Gd(1)#1 | 3.916(3) |
| Gd(2)-O(7)#4 | 2.396(7) | | |
| O(11)#1-Gd(1)-O(11) | 69.2(3) | O(7)#4-Gd(2)-O(12) | 128.4(2) |
| O(11)#1-Gd(1)-O(12) | 129.3(3) | O(7)-Gd(2)-O(8)#3 | 140.2(2) |

| | | | |
|---|---|---|---|
| O(11)-Gd(1)-O(12) | 72.7(3) | O(8)-Gd(2)-O(8)#3 | 69.5(3) |
| O(11)#1-Gd(1)-O(13) | 80.3(2) | O(9)#3-Gd(2)-O(8)#3 | 69.2(3) |
| O(11)-Gd(1)-O(13) | 77.9(2) | O(13)-Gd(2)-O(8)#3 | 83.9(2) |
| O(12)-Gd(1)-O(13) | 59.8(2) | O(7)#4-Gd(2)-O(8)#3 | 75.5(3) |
| O(11)#1-Gd(1)-O(1) | 139.2(2) | O(12)-Gd(2)-O(8)#3 | 129.2(3) |
| O(11)-Gd(1)-O(1) | 95.6(2) | O(7)-Gd(2)-O(4) | 81.3(3) |
| O(12)-Gd(1)-O(1) | 75.7(2) | O(8)-Gd(2)-O(4) | 90.1(3) |
| O(13)-Gd(1)-O(1) | 135.1(2) | O(9)#3-Gd(2)-O(4) | 77.8(2) |
| O(11)#1-Gd(1)-O(9)#2 | 76.9(3) | O(13)-Gd(2)-O(4) | 135.1(2) |
| O(11)-Gd(1)-O(9)#2 | 145.7(2) | O(7)#4-Gd(2)-O(4) | 124.1(3) |
| O(12)-Gd(1)-O(9)#2 | 137.2(3) | O(12)-Gd(2)-O(4) | 75.3(3) |
| O(13)-Gd(1)-O(9)#2 | 101.7(2) | O(8)#3-Gd(2)-O(4) | 133.1(2) |
| O(1)-Gd(1)-O(9)#2 | 107.1(3) | O(12)-Gd(3)-O(13) | 60.5(2) |
| O(11)#1-Gd(1)-O(7) | 133.5(2) | O(12)-Gd(3)-O(9) | 135.5(3) |
| O(11)-Gd(1)-O(7) | 141.0(2) | O(13)-Gd(3)-O(9) | 99.1(2) |
| O(12)-Gd(1)-O(7) | 69.0(3) | O(12)-Gd(3)-O(10) | 131.9(2) |
| O(13)-Gd(1)-O(7) | 76.7(3) | O(13)-Gd(3)-O(10) | 82.2(2) |
| O(1)-Gd(1)-O(7) | 82.2(2) | O(9)-Gd(3)-O(10) | 75.6(2) |
| O(9)#2-Gd(1)-O(7) | 69.1(2) | O(12)-Gd(3)-O(2)#5 | 74.4(3) |
| O(11)#1-Gd(1)-O(10)#1 | 72.9(2) | O(13)-Gd(3)-O(2)#5 | 133.7(3) |
| O(11)-Gd(1)-O(10)#1 | 96.1(3) | O(9)-Gd(3)-O(2)#5 | 106.2(2) |
| O(12)-Gd(1)-O(10)#1 | 144.0(2) | O(10)-Gd(3)-O(2)#5 | 141.1(3) |
| O(13)-Gd(1)-O(10)#1 | 152.9(2) | O(12)-Gd(3)-O(10)#6 | 144.5(2) |
| O(1)-Gd(1)-O(10)#1 | 71.4(2) | O(13)-Gd(3)-O(10)#6 | 152.7(2) |
| O(9)#2-Gd(1)-O(10)#1 | 68.5(2) | O(9)-Gd(3)-O(10)#6 | 69.2(2) |
| O(7)-Gd(1)-O(10)#1 | 119.5(3) | O(10)-Gd(3)-O(10)#6 | 71.1(2) |
| O(7)-Gd(2)-O(8) | 140.7(3) | O(2)#5-Gd(3)-O(10)#6 | 73.5(3) |
| O(7)-Gd(2)-O(9)#3 | 108.8(3) | O(12)-Gd(3)-O(8) | 68.8(3) |
| O(8)-Gd(2)-O(9)#3 | 106.6(2) | O(13)-Gd(3)-O(8) | 77.6(2) |
| O(7)-Gd(2)-O(13) | 79.7(3) | O(9)-Gd(3)-O(8) | 68.2(3) |
| O(8)-Gd(2)-O(13) | 79.9(2) | O(10)-Gd(3)-O(8) | 134.5(2) |
| O(9)#3-Gd(2)-O(13) | 147.1(2) | O(2)#5-Gd(3)-O(8) | 77.0(2) |
| O(7)-Gd(2)-O(7)#4 | 67.0(3) | O(10)#6-Gd(3)-O(8) | 117.4(2) |
| O(8)-Gd(2)-O(7)#4 | 142.7(3) | O(12)-Gd(3)-O(11) | 70.7(3) |
| O(9)#3-Gd(2)-O(7)#4 | 71.2(2) | O(13)-Gd(3)-O(11) | 75.8(2) |
| O(13)-Gd(2)-O(7)#4 | 84.2(2) | O(9)-Gd(3)-O(11) | 147.1(2) |
| O(7)-Gd(2)-O(12) | 70.8(3) | O(10)-Gd(3)-O(11) | 71.6(2) |
| O(8)-Gd(2)-O(12) | 69.9(3) | O(2)#5-Gd(3)-O(11) | 99.9(2) |
| O(9)#3-Gd(2)-O(12) | 152.9(2) | O(10)#6-Gd(3)-O(11) | 100.3(2) |
| O(13)-Gd(2)-O(12) | 60.0(2) | O(8)-Gd(3)-O(11) | 138.7(3) |

[b]Symmetry codes: (#1) -x+1,-y,-z; ( #2) x+1,y,z; ( #3) -x,-y+1,-z; ( #4) -x+1,-y+1,-z; (#5) x-1,y,z; (#6) -x,-y,-z; (#7) -x+1,-y,-z+1; (#8) -x,-y+1,-z+1

**Table S3** Closest metal-metal distances, selected bond lengths and angles in compound **3**

| **Compound 3[c]** | | | |
|---|---|---|---|
| Er(1)-O(13A) | 1.999(16) | Er(2)-O(9)#1 | 2.340(6) |
| Er(1)-O(10A)#1 | 2.000(15) | Er(2)-O(9) | 2.344(7) |
| Er(1)-O(13A)#2 | 2.203(15) | Er(2)-O(7) | 2.356(6) |
| Er(1)-O(13) | 2.281(12) | Er(2)-O(11)#3 | 2.364(7) |
| Er(1)-O(7) | 2.314(6) | Er(2)-O(4) | 2.399(7) |
| Er(1)-O(9) | 2.360(7) | Er(2)-O(8A) | 2.71(2) |
| Er(1)-O(13)#2 | 2.355(12) | Er(2)-Er(3) | 3.4872(8) |
| Er(1)-O(8) | 2.371(19) | Er(3)-O(8A) | 1.969(18) |
| Er(1)-O(1) | 2.393(7) | Er(3)-O(7) | 2.319(8) |
| Er(1)-O(10)#1 | 2.402(11) | Er(3)-O(12) | 2.328(7) |
| Er(1)-O(12)#2 | 2.408(6) | Er(3)-O(10)#3 | 2.358(11) |
| Er(1)-Er(2) | 3.5057(12) | Er(3)-O(12)#4 | 2.354(7) |
| Er(2)-O(8B) | 1.92(2) | Er(3)-O(8) | 2.353(18) |
| Er(2)-O(10A) | 2.254(17) | Er(3)-O(2)#5 | 2.363(7) |
| Er(2)-O(10) | 2.316(11) | Er(3)-O(13)#2 | 2.381(11) |
| Er(2)-O(11) | 2.316(7) | Er(3)-O(11) | 2.438(6) |
| Er(2)-O(8) | 2.343(19) | Er(3)-O(8B) | 2.609(19) |
| O(13A)-Er(1)-O(10A)#1 | 78.3(6) | O(10)-Er(2)-O(7) | 151.8(3) |
| O(13A)-Er(1)-O(13A)#2 | 51.4(7) | O(11)-Er(2)-O(7) | 71.1(2) |
| O(10A)#1-Er(1)-O(13A)#2 | 129.5(6) | O(8)-Er(2)-O(7) | 60.5(5) |
| O(13A)-Er(1)-O(13) | 15.6(5) | O(9)#1-Er(2)-O(7) | 129.7(2) |
| O(10A)#1-Er(1)-O(13) | 74.2(5) | O(9)-Er(2)-O(7) | 69.0(2) |
| O(13A)#2-Er(1)-O(13) | 58.8(5) | O(8B)-Er(2)-O(11)#3 | 56.8(6) |
| O(13A)-Er(1)-O(7) | 116.1(5) | O(10A)-Er(2)-O(11)#3 | 95.2(4) |
| O(10A)#1-Er(1)-O(7) | 114.1(4) | O(10)-Er(2)-O(11)#3 | 70.2(3) |
| O(13A)#2-Er(1)-O(7) | 87.4(4) | O(11)-Er(2)-O(11)#3 | 69.2(3) |
| O(13)-Er(1)-O(7) | 131.6(4) | O(8)-Er(2)-O(11)#3 | 83.4(5) |
| O(13A)-Er(1)-O(9) | 134.9(4) | O(9)#1-Er(2)-O(11)#3 | 74.1(2) |
| O(10A)#1-Er(1)-O(9) | 61.0(5) | O(9)-Er(2)-O(11)#3 | 141.1(2) |
| O(13A)#2-Er(1)-O(9) | 156.3(4) | O(7)-Er(2)-O(11)#3 | 129.4(3) |
| O(13)-Er(1)-O(9) | 135.0(3) | O(8B)-Er(2)-O(4) | 152.9(6) |
| O(7)-Er(1)-O(9) | 69.4(2) | O(10A)-Er(2)-O(4) | 70.3(4) |
| O(13A)-Er(1)-O(13)#2 | 60.1(5) | O(10)-Er(2)-O(4) | 77.5(3) |
| O(10A)#1-Er(1)-O(13)#2 | 133.4(6) | O(11)-Er(2)-O(4) | 90.6(2) |
| O(13A)#2-Er(1)-O(13)#2 | 15.8(4) | O(8)-Er(2)-O(4) | 134.6(5) |
| O(13)-Er(1)-O(13)#2 | 70.5(4) | O(9)#1-Er(2)-O(4) | 123.7(3) |
| O(7)-Er(1)-O(13)#2 | 71.8(3) | O(9)-Er(2)-O(4) | 79.3(2) |
| O(9)-Er(1)-O(13)#2 | 140.5(3) | O(7)-Er(2)-O(4) | 74.6(2) |
| O(13A)-Er(1)-O(8) | 69.2(6) | O(11)#3-Er(2)-O(4) | 134.8(2) |
| O(10A)#1-Er(1)-O(8) | 68.9(6) | O(8B)-Er(2)-O(8A) | 13.6(7) |
| O(13A)#2-Er(1)-O(8) | 86.4(6) | O(10A)-Er(2)-O(8A) | 150.2(5) |

| | | | |
|---|---|---|---|
| O(13)-Er(1)-O(8) | 82.1(5) | O(10)-Er(2)-O(8A) | 133.2(5) |
| O(7)-Er(1)-O(8) | 60.7(5) | O(11)-Er(2)-O(8A) | 59.4(4) |
| O(9)-Er(1)-O(8) | 78.3(5) | O(8)-Er(2)-O(8A) | 26.5(6) |
| O(13)#2-Er(1)-O(8) | 76.9(5) | O(9)#1-Er(2)-O(8A) | 94.6(4) |
| O(13A)-Er(1)-O(1) | 143.1(4) | O(9)-Er(2)-O(8A) | 105.6(4) |
| O(10A)#1-Er(1)-O(1) | 131.8(5) | O(7)-Er(2)-O(8A) | 70.3(4) |
| O(13A)#2-Er(1)-O(1) | 97.0(4) | O(11)#3-Er(2)-O(8A) | 63.0(4) |
| O(13)-Er(1)-O(1) | 137.0(3) | O(4)-Er(2)-O(8A) | 139.5(4) |
| O(7)-Er(1)-O(1) | 74.8(2) | O(8A)-Er(3)-O(7) | 85.9(7) |
| O(9)-Er(1)-O(1) | 81.8(2) | O(8A)-Er(3)-O(12) | 75.4(6) |
| O(13)#2-Er(1)-O(1) | 94.8(3) | O(7)-Er(3)-O(12) | 132.1(2) |
| O(8)-Er(1)-O(1) | 135.2(5) | O(8A)-Er(3)-O(10)#3 | 67.4(7) |
| O(13A)-Er(1)-O(10)#1 | 86.7(5) | O(7)-Er(3)-O(10)#3 | 136.0(3) |
| O(10A)#1-Er(1)-O(10)#1 | 31.6(5) | O(12)-Er(3)-O(10)#3 | 75.7(3) |
| O(13A)#2-Er(1)-O(10)#1 | 132.3(5) | O(8A)-Er(3)-O(12)#4 | 129.1(7) |
| O(13)-Er(1)-O(10)#1 | 75.3(4) | O(7)-Er(3)-O(12)#4 | 145.0(2) |
| O(7)-Er(1)-O(10)#1 | 137.1(3) | O(12)-Er(3)-O(12)#4 | 69.0(3) |
| O(9)-Er(1)-O(10)#1 | 69.1(3) | O(10)#3-Er(3)-O(12)#4 | 69.2(3) |
| O(13)#2-Er(1)-O(10)#1 | 145.7(4) | O(8A)-Er(3)-O(8) | 31.0(8) |
| O(8)-Er(1)-O(10)#1 | 100.4(5) | O(7)-Er(3)-O(8) | 60.9(5) |
| O(1)-Er(1)-O(10)#1 | 109.3(3) | O(12)-Er(3)-O(8) | 83.4(5) |
| O(13A)-Er(1)-O(12)#2 | 84.5(4) | O(10)#3-Er(3)-O(8) | 98.3(5) |
| O(10A)#1-Er(1)-O(12)#2 | 97.2(5) | O(12)#4-Er(3)-O(8) | 151.6(5) |
| O(13A)#2-Er(1)-O(12)#2 | 84.4(4) | O(8A)-Er(3)-O(2)#5 | 144.8(6) |
| O(13)-Er(1)-O(12)#2 | 70.6(3) | O(7)-Er(3)-O(2)#5 | 74.8(2) |
| O(7)-Er(1)-O(12)#2 | 144.8(2) | O(12)-Er(3)-O(2)#5 | 138.7(2) |
| O(9)-Er(1)-O(12)#2 | 117.2(2) | O(10)#3-Er(3)-O(2)#5 | 107.2(3) |
| O(13)#2-Er(1)-O(12)#2 | 98.6(3) | O(12)#4-Er(3)-O(2)#5 | 73.7(3) |
| O(8)-Er(1)-O(12)#2 | 152.0(5) | O(8)-Er(3)-O(2)#5 | 134.5(6) |
| O(1)-Er(1)-O(12)#2 | 72.3(2) | O(8A)-Er(3)-O(13)#2 | 102.0(6) |
| O(10)#1-Er(1)-O(12)#2 | 67.7(3) | O(7)-Er(3)-O(13)#2 | 71.2(3) |
| O(8B)-Er(2)-O(10A) | 136.9(7) | O(12)-Er(3)-O(13)#2 | 70.3(4) |
| O(8B)-Er(2)-O(10) | 125.1(6) | O(10)#3-Er(3)-O(13)#2 | 146.0(4) |
| O(10A)-Er(2)-O(10) | 32.0(5) | O(12)#4-Er(3)-O(13)#2 | 99.1(3) |
| O(8B)-Er(2)-O(11) | 70.1(6) | O(8)-Er(3)-O(13)#2 | 76.7(5) |
| O(10A)-Er(2)-O(11) | 134.6(4) | O(2)#5-Er(3)-O(13)#2 | 99.3(3) |
| O(10)-Er(2)-O(11) | 105.2(3) | O(8A)-Er(3)-O(11) | 68.6(6) |
| O(8B)-Er(2)-O(8) | 26.8(7) | O(7)-Er(3)-O(11) | 69.6(2) |
| O(10A)-Er(2)-O(8) | 141.1(6) | O(12)-Er(3)-O(11) | 136.4(2) |
| O(10)-Er(2)-O(8) | 147.7(5) | O(10)#3-Er(3)-O(11) | 68.2(3) |
| O(11)-Er(2)-O(8) | 81.2(5) | O(12)#4-Er(3)-O(11) | 117.0(2) |
| O(8B)-Er(2)-O(9)#1 | 81.3(6) | O(8)-Er(3)-O(11) | 78.5(4) |
| O(10A)-Er(2)-O(9)#1 | 58.2(4) | O(2)#5-Er(3)-O(11) | 77.1(2) |
| O(10)-Er(2)-O(9)#1 | 70.9(3) | O(13)#2-Er(3)-O(11) | 140.2(4) |

| | | | |
|---|---|---|---|
| O(11)-Er(2)-O(9)#1 | 141.7(3) | O(8A)-Er(3)-O(8B) | 18.2(8) |
| O(8)-Er(2)-O(9)#1 | 84.5(5) | O(7)-Er(3)-O(8B) | 68.8(5) |
| O(8B)-Er(2)-O(9) | 102.9(6) | O(12)-Er(3)-O(8B) | 91.9(5) |
| O(10A)-Er(2)-O(9) | 78.0(4) | O(10)#3-Er(3)-O(8B) | 78.6(5) |
| O(10)-Er(2)-O(9) | 109.9(3) | O(12)#4-Er(3)-O(8B) | 145.6(5) |
| O(11)-Er(2)-O(9) | 140.1(2) | O(8)-Er(3)-O(8B) | 24.2(6) |
| O(8)-Er(2)-O(9) | 79.2(5) | O(2)#5-Er(3)-O(8B) | 129.3(5) |
| O(9)#1-Er(2)-O(9) | 69.9(3) | O(13)#2-Er(3)-O(8B) | 100.9(5) |
| O(8B)-Er(2)-O(7) | 81.0(6) | O(11)-Er(3)-O(8B) | 58.0(4) |
| O(10A)-Er(2)-O(7) | 135.3(4) | | |

[c]Symmetry codes: (#1) -x,-y,-z+1; (#2) -x,-y+1,-z+1;(#3) -x+1,-y,-z+1; (#4) -x+1,-y+1,-z+1; (#5) x+1,y,z; (#6) x-1,y,z; (#7) -x,-y+1,-z; (#8) -x+1,-y,-z

**Table S4** Closest metal-metal distances, selected bond lengths and angles in compound **4**

| **Compound 4[d]** | | | |
|---|---|---|---|
| Yb(1)-O(10) | 2.272(8) | Yb(2)-O(9)#4 | 2.371(8) |
| Yb(1)-O(11) | 2.280(8) | Yb(2)-O(11) | 2.369(8) |
| Yb(1)-O(11)#1 | 2.287(8) | Yb(2)-O(8)#3 | 2.389(8) |
| Yb(1)-O(9)#2 | 2.298(8) | Yb(2)-S(2) | 3.451(4) |
| Yb(1)-O(10)#2 | 2.316(8) | Yb(2)-Yb(3) | 3.459(2) |
| Yb(1)-O(12) | 2.339(8) | Yb(2)-Yb(3)#4 | 3.671(2) |
| Yb(1)-O(13) | 2.367(8) | Yb(3)-O(13) | 2.277(8) |
| Yb(1)-O(1) | 2.408(9) | Yb(3)-O(8) | 2.310(8) |
| Yb(1)-Yb(3) | 3.4408(19) | Yb(3)-O(9) | 2.324(8) |
| Yb(1)-Yb(2) | 3.4643(17) | Yb(3)-O(12) | 2.335(8) |
| Yb(1)-Yb(2)#1 | 3.771(2) | Yb(3)-O(6)#5 | 2.345(9) |
| Yb(1)-Yb(1)#1 | 3.780(2) | Yb(3)-O(8)#6 | 2.384(8) |
| Yb(2)-O(7)#3 | 2.275(8) | Yb(3)-O(7) | 2.417(8) |
| Yb(2)-O(13) | 2.299(8) | Yb(3)-O(10) | 2.441(8) |
| Yb(2)-O(7) | 2.316(8) | Yb(3)-Yb(2)#5 | 3.671(2) |
| Yb(2)-O(12) | 2.354(8) | Yb(3)-Yb(2)#3 | 3.8031(17) |
| Yb(2)-O(4) | 2.365(9) | | |
| O(10)-Yb(1)-O(11) | 141.6(3) | O(4)-Yb(2)-O(9)#4 | 109.2(3) |
| O(10)-Yb(1)-O(11)#1 | 142.5(3) | O(7)#3-Yb(2)-O(11) | 133.7(3) |
| O(11)-Yb(1)-O(11)#1 | 68.3(3) | O(13)-Yb(2)-O(11) | 69.8(3) |
| O(10)-Yb(1)-O(9)#2 | 104.2(3) | O(7)-Yb(2)-O(11) | 141.1(3) |
| O(11)-Yb(1)-O(9)#2 | 109.3(3) | O(12)-Yb(2)-O(11) | 77.8(3) |
| O(11)#1-Yb(1)-O(9)#2 | 71.3(3) | O(4)-Yb(2)-O(11) | 83.1(3) |
| O(10)-Yb(1)-O(10)#2 | 67.9(3) | O(9)#4-Yb(2)-O(11) | 68.7(3) |
| O(11)-Yb(1)-O(10)#2 | 141.7(3) | O(7)#3-Yb(2)-O(8)#3 | 72.4(3) |
| O(11)#1-Yb(1)-O(10)#2 | 75.9(3) | O(13)-Yb(2)-O(8)#3 | 142.7(3) |
| O(9)#2-Yb(1)-O(10)#2 | 70.0(3) | O(7)-Yb(2)-O(8)#3 | 95.7(3) |
| O(10)-Yb(1)-O(12) | 82.0(3) | O(12)-Yb(2)-O(8)#3 | 151.8(3) |

| | | | |
|---|---|---|---|
| O(11)-Yb(1)-O(12) | 79.9(3) | O(4)-Yb(2)-O(8)#3 | 71.4(3) |
| O(11)#1-Yb(1)-O(12) | 84.1(3) | O(9)#4-Yb(2)-O(8)#3 | 69.1(3) |
| O(9)#2-Yb(1)-O(12) | 147.1(3) | O(11)-Yb(2)-O(8)#3 | 118.8(3) |
| O(10)#2-Yb(1)-O(12) | 83.3(3) | O(13)-Yb(3)-O(8) | 131.9(3) |
| O(10)-Yb(1)-O(13) | 71.5(3) | O(13)-Yb(3)-O(9) | 136.2(3) |
| O(11)-Yb(1)-O(13) | 70.1(3) | O(8)-Yb(3)-O(9) | 76.6(3) |
| O(11)#1-Yb(1)-O(13) | 129.5(3) | O(13)-Yb(3)-O(12) | 62.8(3) |
| O(9)#2-Yb(1)-O(13) | 151.4(3) | O(8)-Yb(3)-O(12) | 81.5(3) |
| O(10)#2-Yb(1)-O(13) | 128.9(3) | O(9)-Yb(3)-O(12) | 98.2(3) |
| O(12)-Yb(1)-O(13) | 61.4(3) | O(13)-Yb(3)-O(6)#5 | 73.3(3) |
| O(10)-Yb(1)-O(1) | 89.6(3) | O(8)-Yb(3)-O(6)#5 | 140.3(3) |
| O(11)-Yb(1)-O(1) | 79.6(3) | O(9)-Yb(3)-O(6)#5 | 106.7(3) |
| O(11)#1-Yb(1)-O(1) | 124.1(3) | O(12)-Yb(3)-O(6)#5 | 134.8(3) |
| O(9)#2-Yb(1)-O(1) | 78.4(3) | O(13)-Yb(3)-O(8)#6 | 142.8(3) |
| O(10)#2-Yb(1)-O(1) | 134.2(3) | O(8)-Yb(3)-O(8)#6 | 71.0(3) |
| O(12)-Yb(1)-O(1) | 134.4(3) | O(9)-Yb(3)-O(8)#6 | 70.0(3) |
| O(13)-Yb(1)-O(1) | 73.4(3) | O(12)-Yb(3)-O(8)#6 | 151.7(3) |
| O(7)#3-Yb(2)-O(13) | 130.5(3) | O(6)#5-Yb(3)-O(8)#6 | 73.3(3) |
| O(7)#3-Yb(2)-O(7) | 70.9(3) | O(13)-Yb(3)-O(7) | 70.4(3) |
| O(13)-Yb(2)-O(7) | 71.8(3) | O(8)-Yb(3)-O(7) | 71.3(3) |
| O(7)#3-Yb(2)-O(12) | 79.8(3) | O(9)-Yb(3)-O(7) | 147.9(3) |
| O(13)-Yb(2)-O(12) | 62.1(3) | O(12)-Yb(3)-O(7) | 77.4(3) |
| O(7)-Yb(2)-O(12) | 79.1(3) | O(6)#5-Yb(3)-O(7) | 98.0(3) |
| O(7)#3-Yb(2)-O(4) | 138.0(3) | O(8)#6-Yb(3)-O(7) | 98.7(3) |
| O(13)-Yb(2)-O(4) | 74.1(3) | O(13)-Yb(3)-O(10) | 70.1(3) |
| O(7)-Yb(2)-O(4) | 92.4(3) | O(8)-Yb(3)-O(10) | 135.5(3) |
| O(12)-Yb(2)-O(4) | 136.0(3) | O(9)-Yb(3)-O(10) | 67.5(3) |
| O(7)#3-Yb(2)-O(9)#4 | 76.2(3) | O(12)-Yb(3)-O(10) | 78.6(3) |
| O(13)-Yb(2)-O(9)#4 | 137.5(3) | O(6)#5-Yb(3)-O(10) | 77.1(3) |
| O(7)-Yb(2)-O(9)#4 | 146.7(3) | O(8)#6-Yb(3)-O(10) | 117.1(3) |
| O(12)-Yb(2)-O(9)#4 | 100.2(3) | O(7)-Yb(3)-O(10) | 139.8(3) |

[d]Symmetry codes: (#1) -x-2,-y+2,-z+1; (#2) -x-3,-y+2,-z+1; (#3) -x-2,-y+1,-z+1; (#4) x+1,y,z; (#5) x-1,y,z; (#6) -x-3,-y+1,-z+1; (#7) -x-3,-y+2,-z+2; (#8) -x-2,-y+1,-z+2

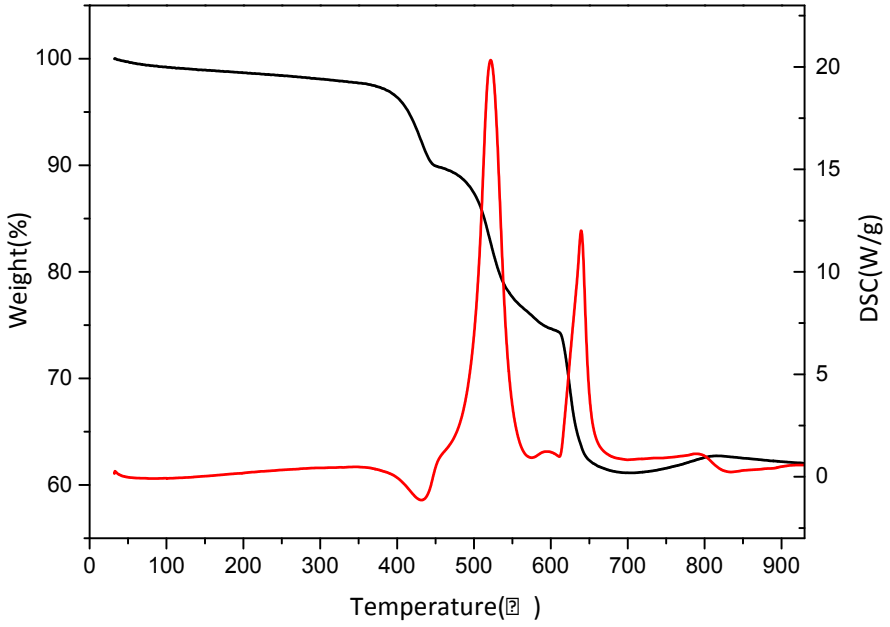


**Fig. S5** TGA-DSC curves of compound **1.**

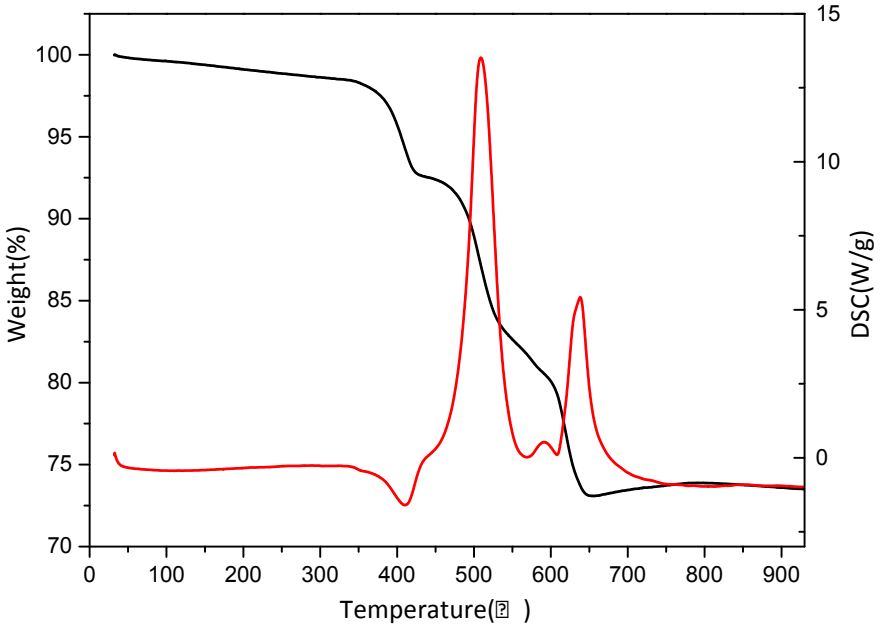


**Fig. S6** TGA-DSC curves of compound **2.**

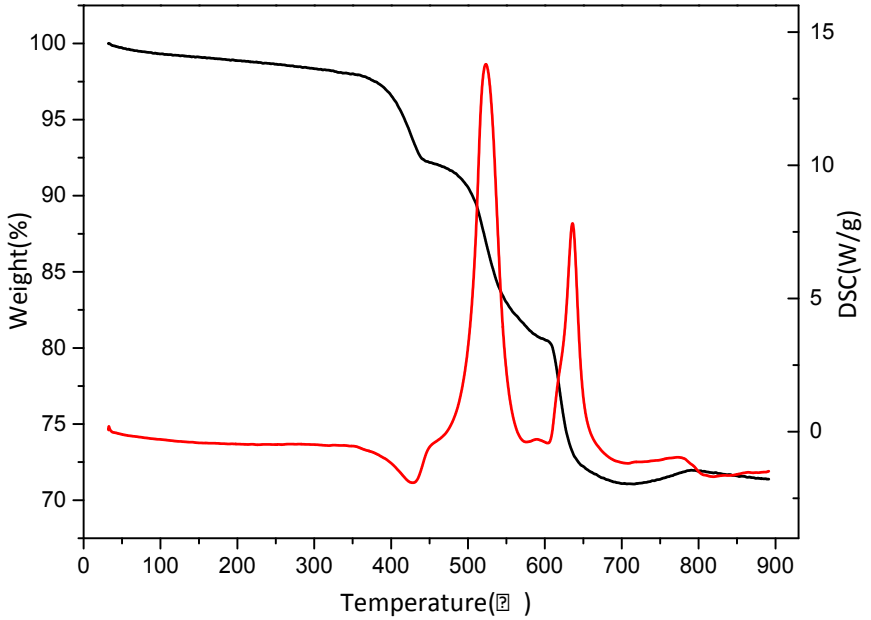


**Fig. S7** TGA-DSC curves of compound **3.**

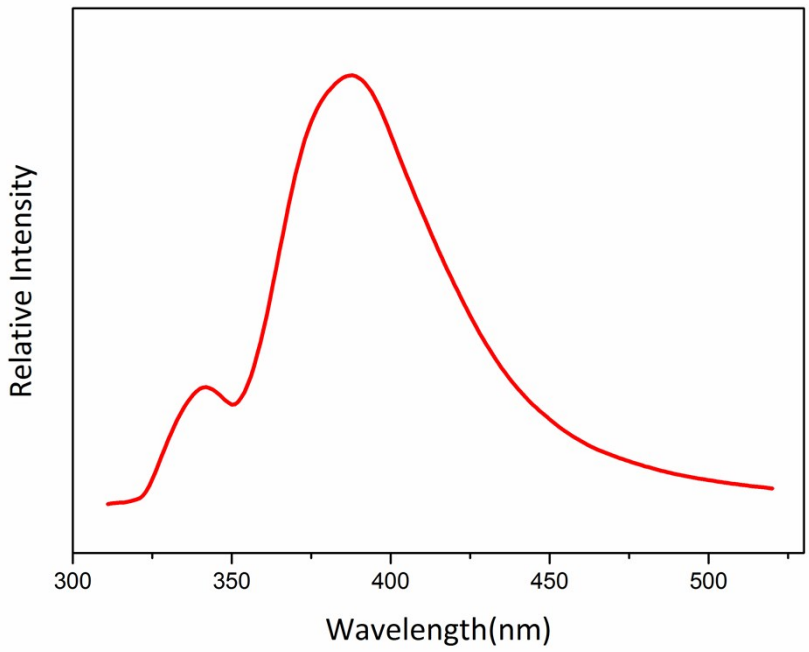


**Fig. S8** The emission spectra of 1,5-NDS ligand.

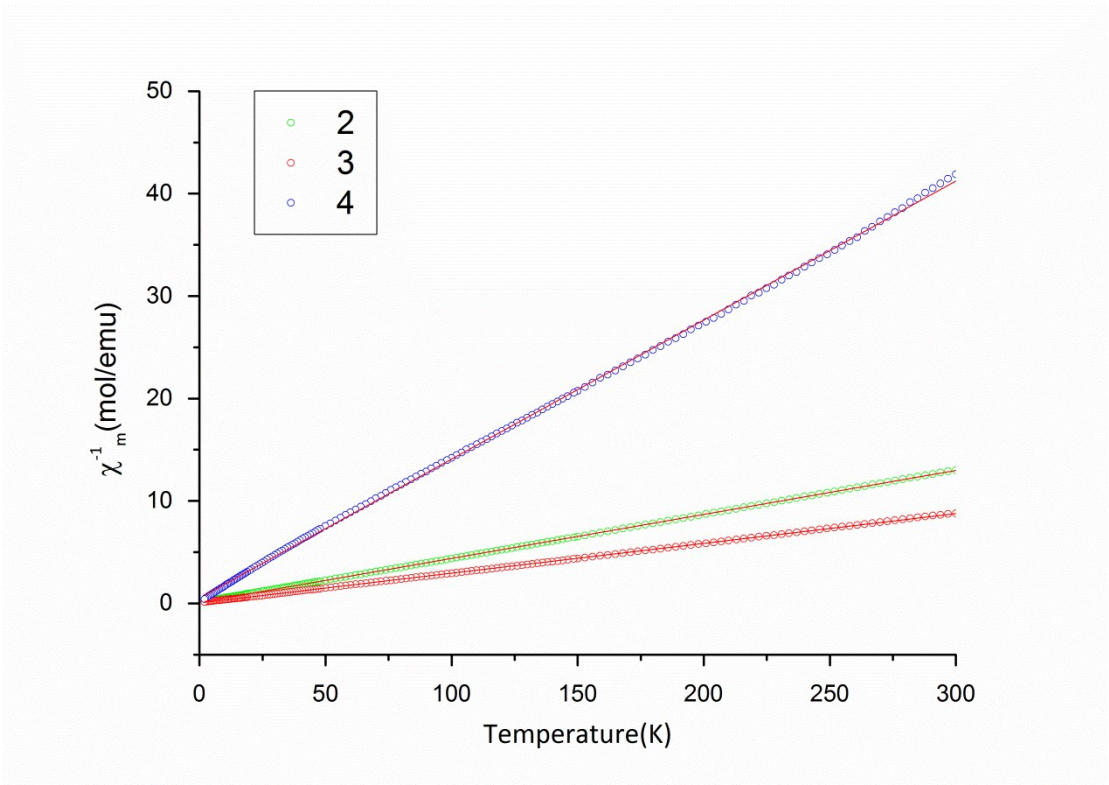


**Fig. S9** The Curie-Weiss fitting of the $\chi^{-1}_{m}$-T data for compounds **2**-**4**.