

Supporting Information

Rare Earth Metal Oxalatophosphonates: Syntheses, Structure Diversity and Photoluminescence Properties

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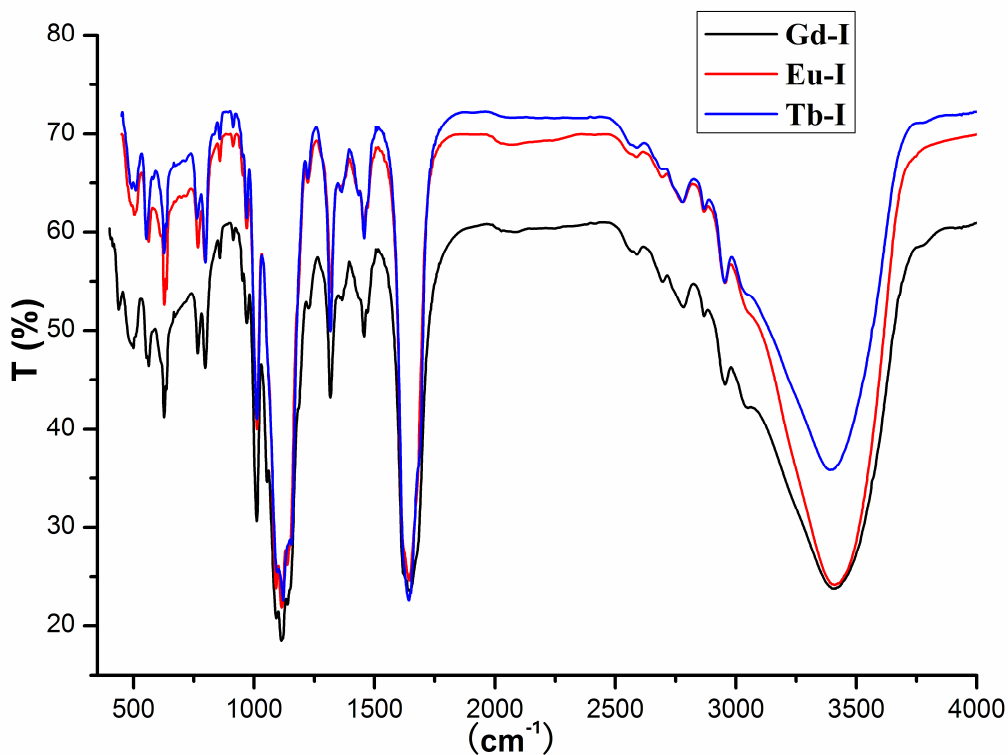


Figure S1. FT-IR spectra for Compounds **1** (black), **2** (red) and **3** (blue).

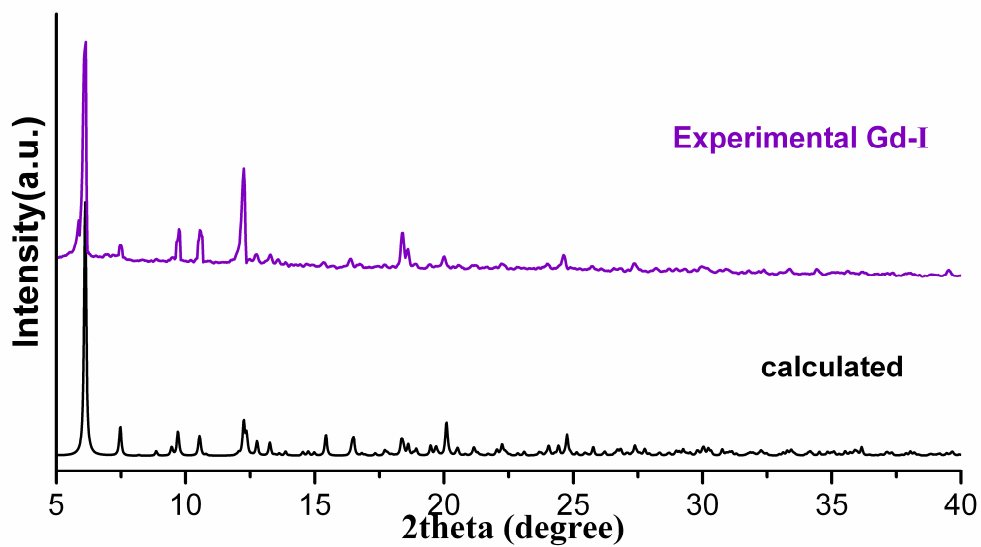


Figure S2. Calculated and experimental XRD powder patterns of compound **1**.

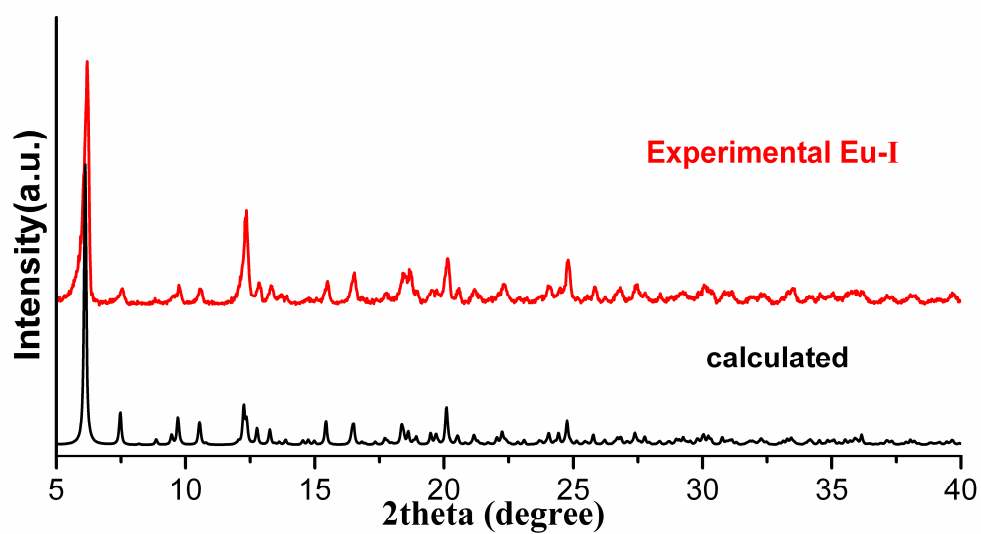


Figure S3. A comparison of the calculated powder pattern of compound **1** (black) and experimental XRD powder pattern of compound **2** (red). The purity of compound **2** can be confirmed.

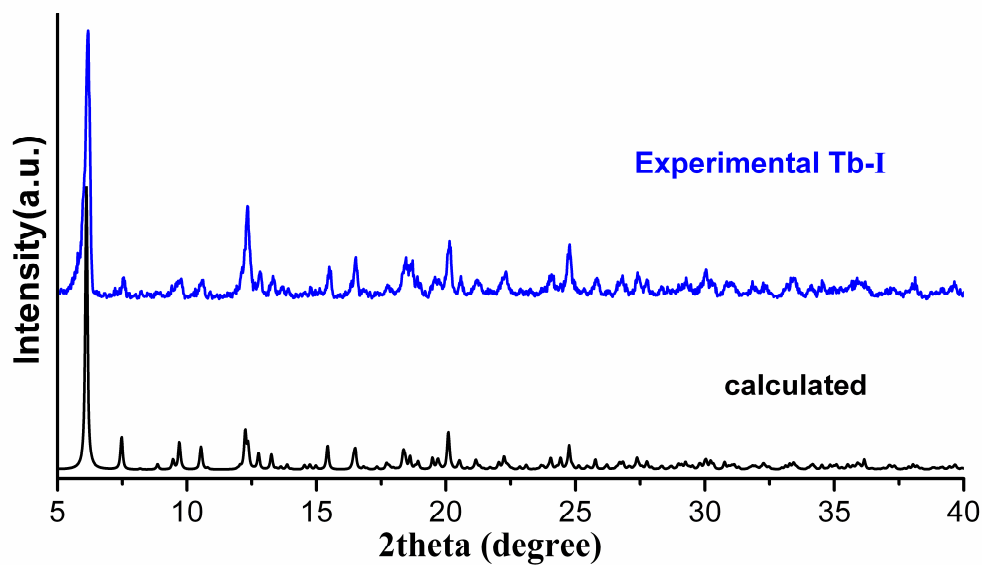


Figure S4. A comparison of the calculated powder pattern of compound **1** (black) and experimental XRD powder pattern of compound **3** (green). The purity of compound **3** can be confirmed.

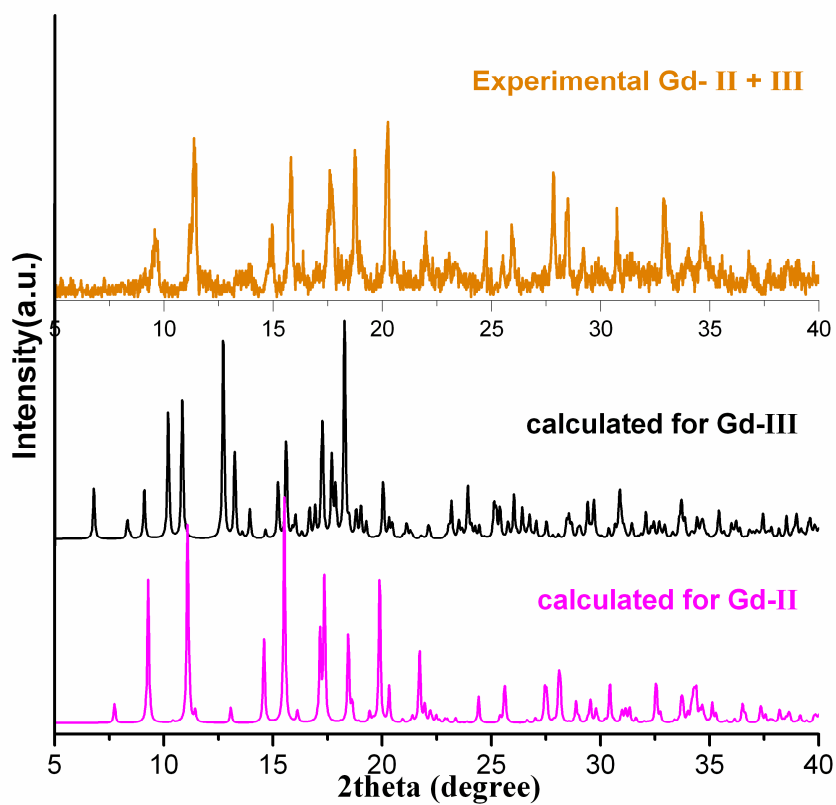


Figure S5. Calculated and experimental XRD powder patterns of compounds **4** and **5**.

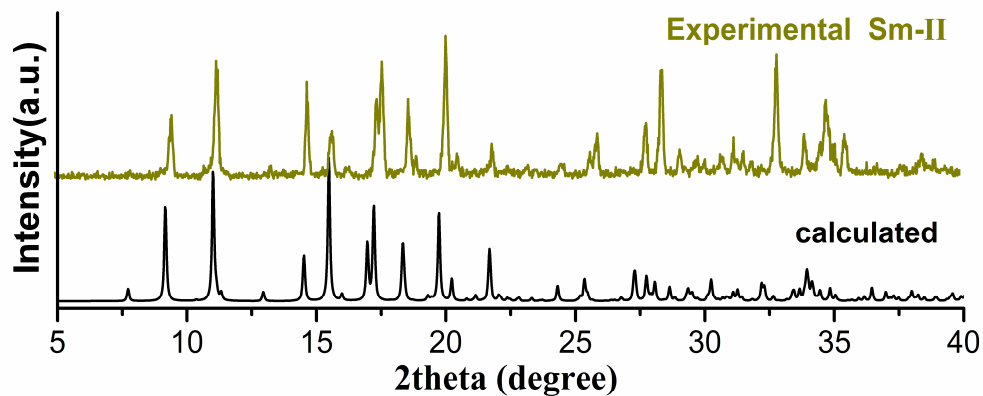


Figure S6. Calculated and experimental XRD powder patterns of compound **6**.

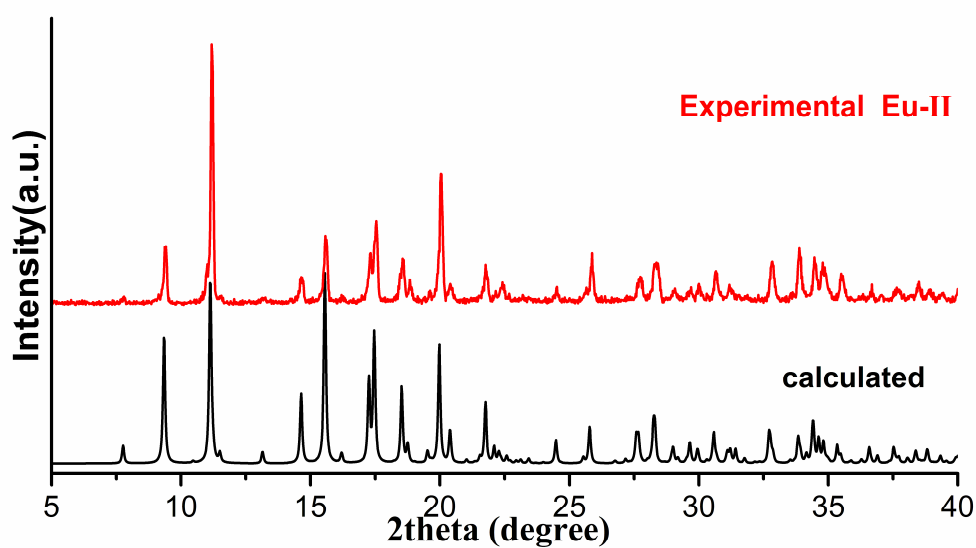


Figure S7. Calculated and experimental XRD powder patterns of compound **7**.

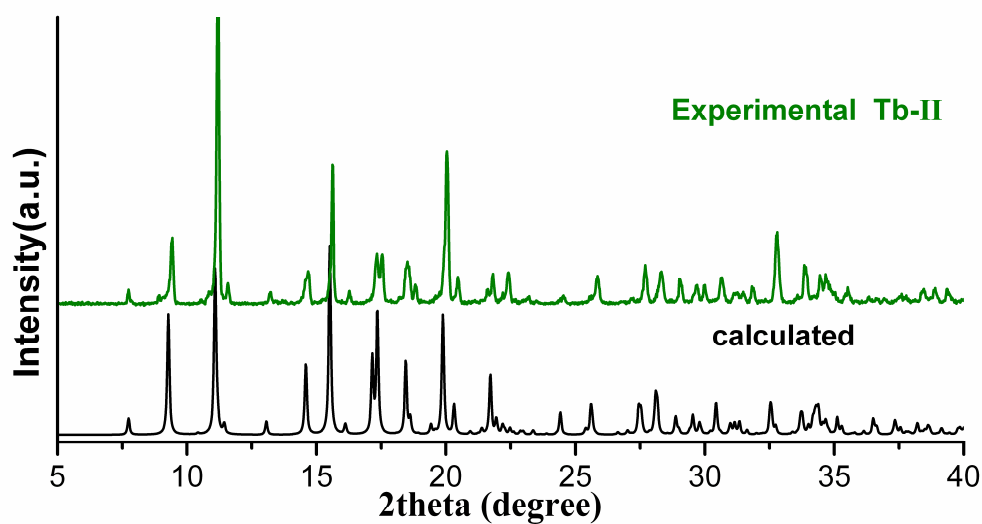


Figure S8. Calculated and experimental XRD powder patterns of compound **8**.

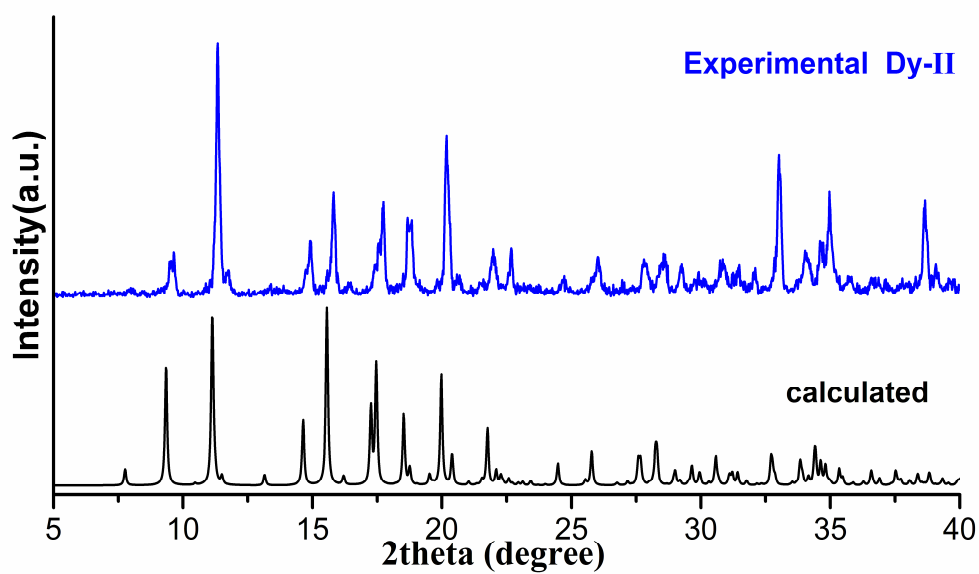


Figure S9. Calculated and experimental XRD powder patterns of compound **9**.

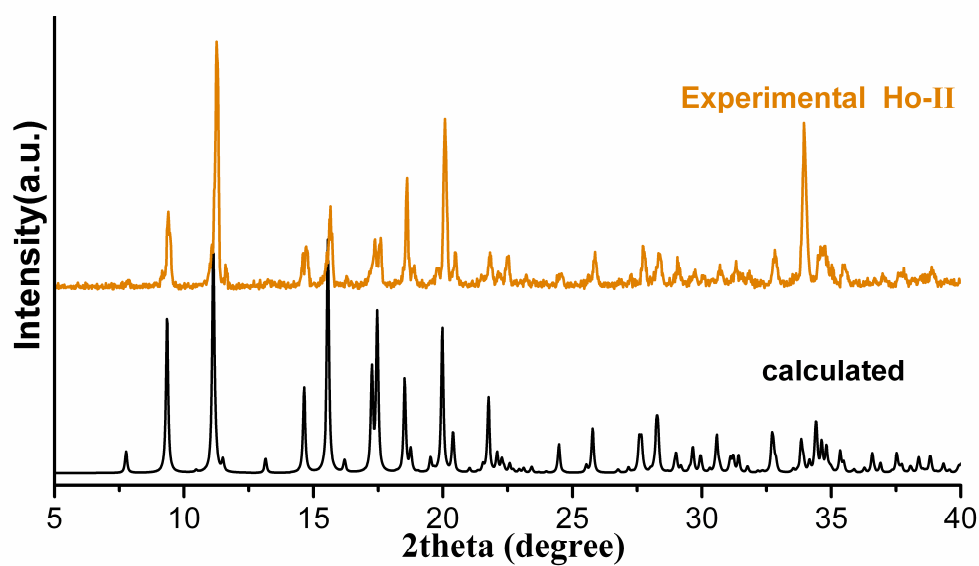


Figure S10. Calculated and experimental XRD powder patterns of compound **10**.

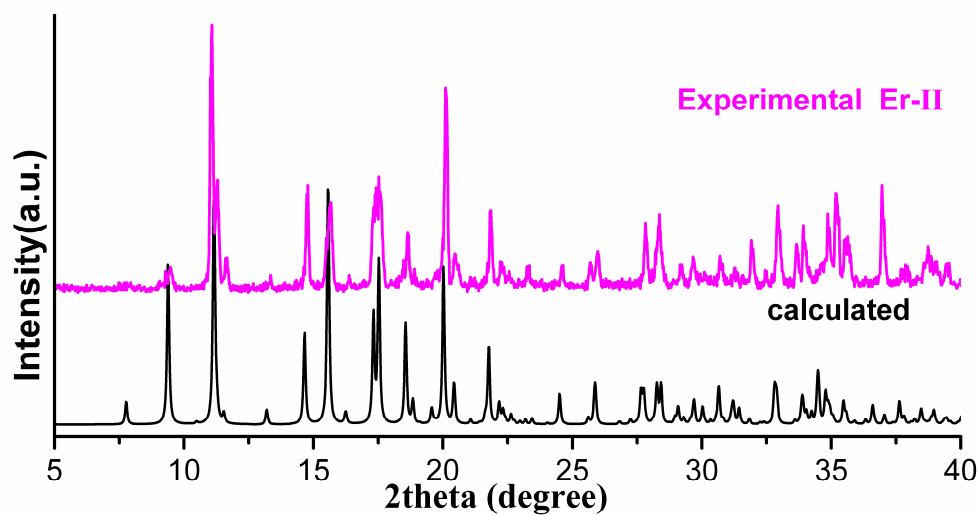


Figure S11. Calculated and experimental XRD powder patterns of compound **11**.

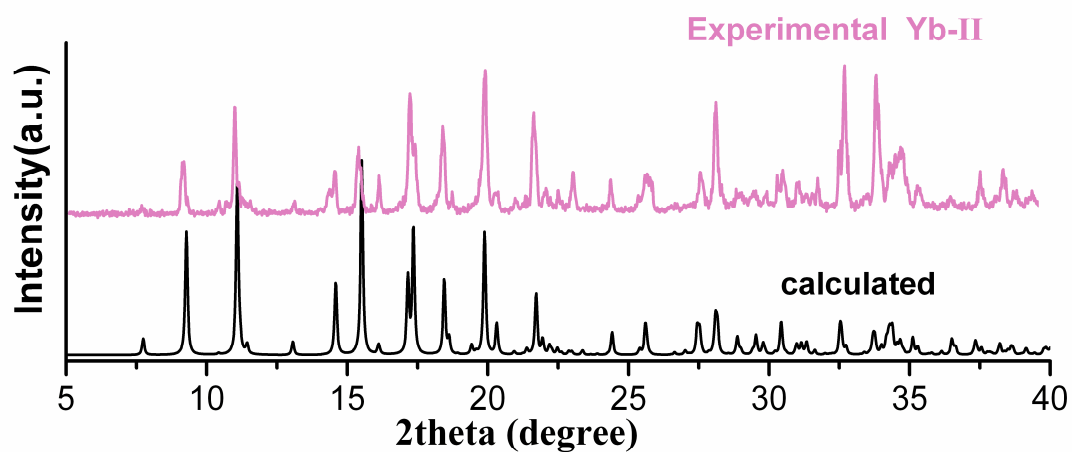


Figure S12. Calculated and experimental XRD powder patterns of compound **12**.

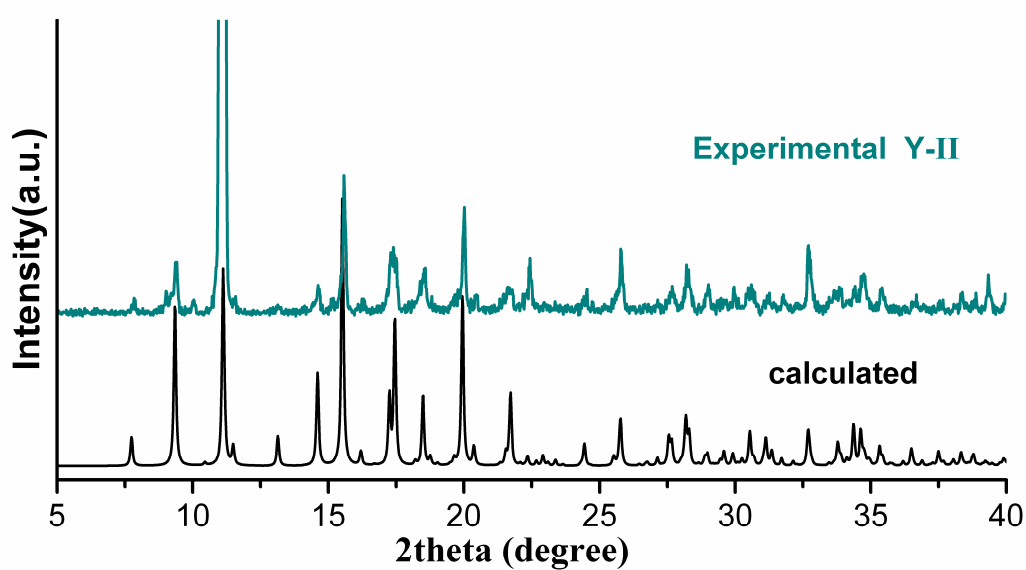


Figure S13. Calculated and experimental XRD powder patterns of compound **13**.

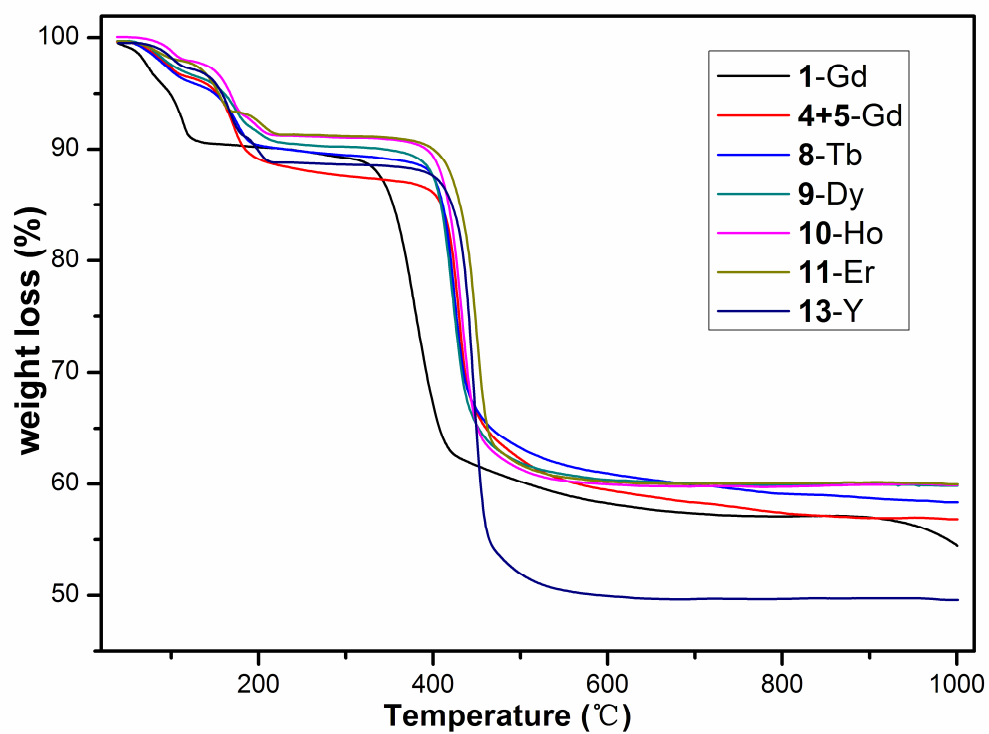
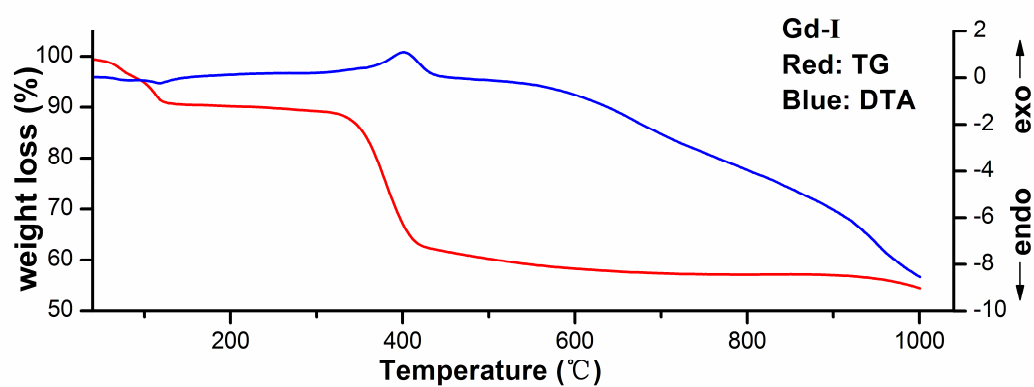
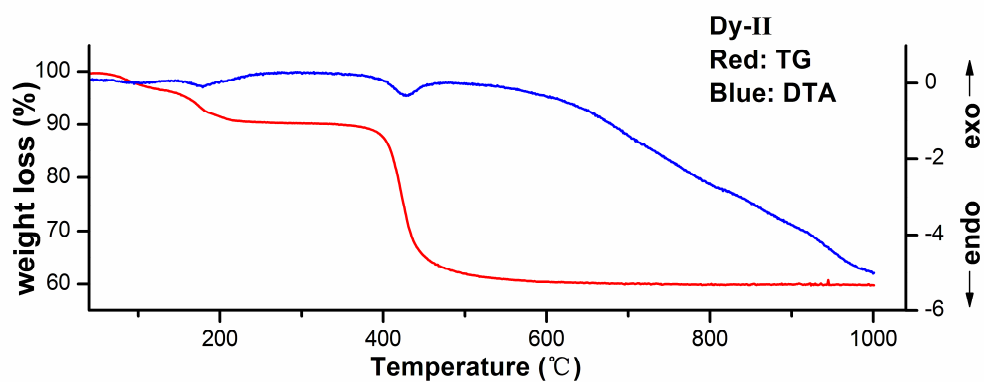


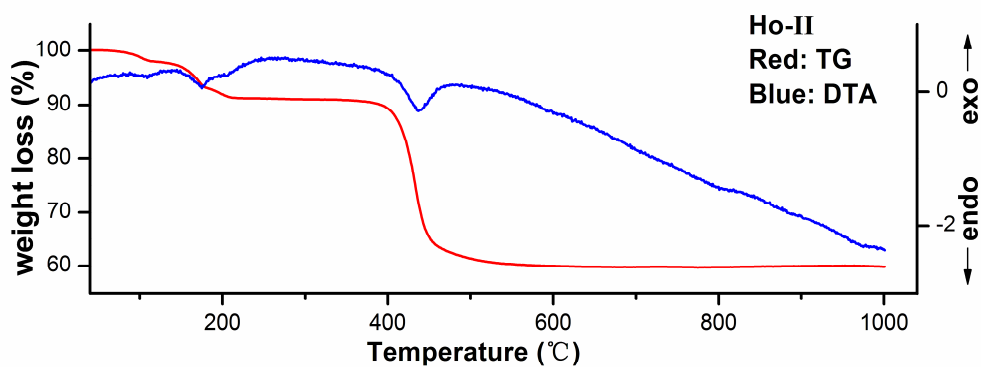
Figure S14. Thermogravimetric analysis (TGA) curves of some of the compounds selected from **1-13**.



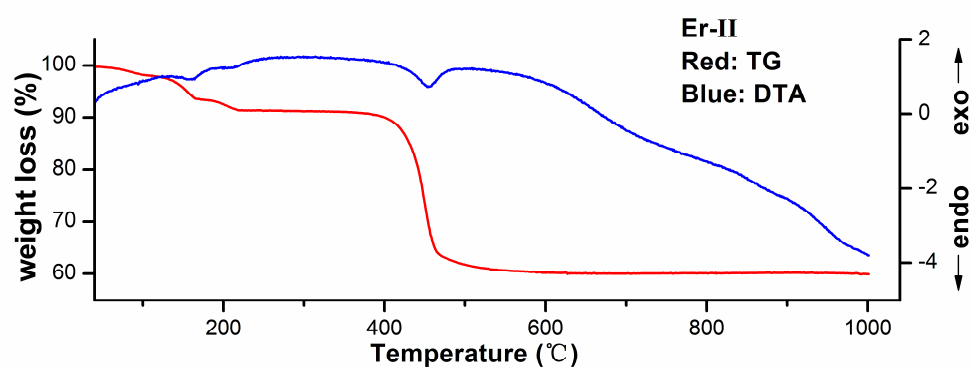
(a)



(b)



(c)



(d)

Figure S15. TGA and DTA curves of compounds **1(a)**, **9(b)**, **10(c)** and **11(d)**.

Table S1. Selected bond lengths [Å] for compounds **6-13**.**Compound 6**

Sm(1)-O(1)	2.282(4)	Sm(1)-O(3)#1	2.392(3)
Sm(1)-O(14)	2.398(3)	Sm(1)-O(8)	2.434(4)
Sm(1)-O(6)	2.457(4)	Sm(1)-O(10)	2.470(3)
Sm(1)-O(4)	2.470(4)	Sm(1)-O(15)	2.495(4)
Sm(2)-O(2)	2.275(3)	Sm(2)-O(5)#2	2.388(4)
Sm(2)-O(11)#3	2.423(4)	Sm(2)-O(12)	2.433(3)
Sm(2)-O(7)#2	2.439(4)	Sm(2)-O(9)#3	2.443(4)
Sm(2)-O(13)#4	2.463(4)	Sm(2)-O(16)	2.512(4)
P(1)-O(1)	1.511(4)	P(1)-O(3)	1.515(3)
P(1)-O(2)	1.516(4)		

Symmetry codes: for **6** #1 -x+1,-y+1,-z+1 #2 -x,-y+2,-z+1 #3 -x,-y+1,-z+1 #4 -x,-y+1,-z+2**Compound 7**

Eu(1)-O(2)	2.258(4)	Eu(1)-O(10)	2.374(4)
Eu(1)-O(5)#1	2.414(4)	Eu(1)-O(13)#2	2.418(4)
Eu(1)-O(7)#1	2.429(4)	Eu(1)-O(8)	2.429(4)
Eu(1)-O(12)	2.452(4)	Eu(1)-O(14)	2.509(5)
Eu(2)-O(1)	2.271(4)	Eu(2)-O(3)#3	2.385(4)
Eu(2)-O(15)	2.390(4)	Eu(2)-O(6)	2.421(4)
Eu(2)-O(9)#4	2.442(4)	Eu(2)-O(4)	2.463(4)
Eu(2)-O(11)#4	2.469(5)	Eu(2)-O(16)	2.488(5)
P(1)-O(1)	1.511(4)	P(1)-O(3)	1.512(4)
P(1)-O(2)	1.517(4)		

Symmetry codes: for **7** #1 -x+1,-y+1,-z+1 #2 -x+1,-y+1,-z #3 -x,-y+1,-z+1 #4 -x+1,-y,-z+1**Compound 8**

Tb(1)-O(2)	2.243(4)	Tb(1)-O(5)#1	2.363(5)
Tb(1)-O(9)#2	2.389(4)	Tb(1)-O(13)#3	2.388(5)

Tb(1)-O(7)#1	2.399(4)	Tb(1)-O(11)#2	2.407(4)
Tb(1)-O(12)	2.430(5)	Tb(1)-O(16)	2.481(6)
Tb(2)-O(1)	2.244(5)	Tb(2)-O(3)#4	2.355(4)
Tb(2)-O(15)	2.365(4)	Tb(2)-O(10)	2.400(5)
Tb(2)-O(6)	2.421(5)	Tb(2)-O(8)	2.440(4)
Tb(2)-O(4)	2.448(5)	Tb(2)-O(14)	2.457(5)
P(1)-O(2)	1.512(5)	P(1)-O(1)	1.511(5)
P(1)-O(3)	1.517(4)		

Symmetry codes: for **8** #1 -x+1,-y,-z+1 #2 -x+1,-y+1,-z+1 #3 -x+1,-y+1,-z #4 -x,-y+1,-z+1

Compound 9

Dy(1)-O(3)#1	2.234(3)	Dy(1)-O(1)	2.341(3)
Dy(1)-O(15)	2.349(3)	Dy(1)-O(9)#2	2.397(3)
Dy(1)-O(4)	2.404(3)	Dy(1)-O(11)#2	2.434(3)
Dy(1)-O(6)	2.439(3)	Dy(1)-O(14)	2.450(4)
Dy(2)-O(2)#3	2.233(3)	Dy(2)-O(7)	2.346(3)
Dy(2)-O(10)	2.383(3)	Dy(2)-O(13)#4	2.382(3)
Dy(2)-O(8)	2.393(3)	Dy(2)-O(5)	2.397(3)
Dy(2)-O(12)	2.418(3)	Dy(2)-O(16)	2.470(4)
P(1)-O(3)	1.511(3)	P(1)-O(2)	1.514(3)
P(1)-O(1)	1.518(3)		

Symmetry codes: for **9** #1 -x+1,-y+2,-z #2 x,y+1,z #3 x+1,y-1,z #4 -x+2,-y,-z+1.

Compound 10

Ho(1)-O(1)	2.230(5)	Ho(1)-O(11)	2.341(5)
Ho(1)-O(13)#1	2.369(5)	Ho(1)-O(7)#2	2.372(5)
Ho(1)-O(5)#2	2.385(5)	Ho(1)-O(9)	2.387(5)
Ho(1)-O(12)	2.405(5)	Ho(1)-O(16)	2.469(6)
Ho(2)-O(3)#3	2.232(5)	Ho(2)-O(2)	2.335(5)
Ho(2)-O(15)	2.349(5)	Ho(2)-O(4)	2.376(5)
Ho(2)-O(8)#4	2.403(5)	Ho(2)-O(6)	2.419(5)

Ho(2)-O(10)#4	2.426(6)	Ho(2)-O(14)	2.435(6)
P(1)-O(3)	1.498(6)	P(1)-O(1)	1.510(5)
P(1)-O(2)	1.516(5)		
Symmetry codes: for 10 #1 -x+2,-y,-z+1 #2 x-1,y,z #3 -x+3,-y,-z #4 x+1,y-1,z.			

Compound 11

Er(1)-O(1)	2.214(5)	Er(1)-O(8)	2.317(5)
Er(1)-O(4)	2.355(5)	Er(1)-O(12)#1	2.361(5)
Er(1)-O(6)	2.362(5)	Er(1)-O(10)	2.363(6)
Er(1)-O(13)	2.393(5)	Er(1)-O(14)	2.446(6)
Er(2)-O(2)	2.214(6)	Er(2)-O(3)#2	2.319(5)
Er(2)-O(15)	2.332(5)	Er(2)-O(7)#3	2.368(5)
Er(2)-O(11)#4	2.372(6)	Er(2)-O(16)	2.407(6)
Er(2)-O(5)#3	2.412(6)	Er(2)-O(9)#4	2.420(6)
P(1)-O(2)	1.507(6)	P(1)-O(1)	1.507(6)
P(1)-O(3)	1.516(5)		
Symmetry codes: for 11 #1 -x,-y,-z+2 #2 -x+1,-y,-z+1 #3 -x,-y,-z+1 #4 -x,-y+1,-z+1.			

Compound 12

Yb(1)-O(1)	2.170(6)	Yb(1)-O(3)#1	2.278(6)
Yb(1)-O(14)	2.291(6)	Yb(1)-O(10)	2.349(6)
Yb(1)-O(4)	2.361(6)	Yb(1)-O(8)	2.401(6)
Yb(1)-O(15)	2.410(8)	Yb(1)-O(6)	2.421(8)
Yb(2)-O(2)	2.186(6)	Yb(2)-O(7)#2	2.315(7)
Yb(2)-O(12)	2.328(7)	Yb(2)-O(9)#3	2.342(6)
Yb(2)-O(11)#3	2.351(6)	Yb(2)-O(13)#4	2.357(6)
Yb(2)-O(5)#2	2.376(6)	Yb(2)-O(16)	2.460(7)
P(1)-O(2)	1.519(6)	P(1)-O(1)	1.522(6)
P(1)-O(3)	1.528(6)		
Symmetry codes: for 12 #1 -x+2,-y+1,-z+1 #2 -x+1,-y+2,-z+1 #3 -x+1,-y+1,-z+1 #4 -x+1,-y+1,-z+2.			

Compound 13

Y(1)-O(2)	2.222(3)	Y(1)-O(9)#1	2.336(3)
Y(1)-O(13)#2	2.369(3)	Y(1)-O(6)	2.372(3)
Y(1)-O(11)#1	2.383(3)	Y(1)-O(4)	2.386(3)
Y(1)-O(12)	2.411(3)	Y(1)-O(16)	2.468(4)
Y(2)-O(1)	2.220(3)	Y(2)-O(3)#3	2.327(3)
Y(2)-O(14)	2.345(4)	Y(2)-O(5)#4	2.386(3)
Y(2)-O(10)	2.395(4)	Y(2)-O(7)#4	2.420(3)
Y(2)-O(15)	2.446(4)	Y(2)-O(8)	2.435(4)
P(1)-O(1)	1.511(4)	P(1)-O(2)	1.513(3)
P(1)-O(3)	1.523(3)		

Symmetry codes: for **13** #1 -x+1,-y+2,-z #2 -x+1,-y+1,-z+1 #3 -x+2,-y+1,-z #4
-x+1,-y+1,-z.
