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Supporting Information

Syntheses, structures and properties of three-dimensional lanthanide frameworks constructed with trigonal anti-prismatic lanthanide cluster

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Table S1 Selected Bond Distances (Å) and Bond Angles (deg) for **1.**

bond			
Gd(1)-O(1)	2.401(4)	Gd(2)-O(6)#5	2.479(5)
Gd(1)-O(1)#1	2.529(4)	Gd(2)-O(3)	2.512(5)
Gd(1)-O(3)	2.311(5)	Gd(2)-O(3)#5	2.512(5)
Gd(1)-O(4)	2.425(4)	Gd(2)-N(2)	2.566(7)
Gd(1)-O(4)#2	2.480(4)	Gd(2)-N(2)#5	2.567(7)
Gd(1)-O(6)	2.311(4)	Gd(2)-N(1)	2.666(6)
Gd(1)-O(7)	2.319(2)	O(1)-Gd(1)#6	2.529(4)
Gd(1)-Gd(1)#2	3.8402(5)	O(4)-Gd(1)#3	2.480(4)
Gd(1)-Gd(2)	4.0005(3)	O(7)-Gd(1)#2	2.319(2)
Gd(2)-O(6)	2.479(5)		
angle			
Gd(1)#2-Gd(1)-Gd(1)#3	60	N(2)#5-Gd(2)-N(1)#5	136.3(2)
O(1)-Gd(1)-O(1)#1	73.99(7)	N(2)-Gd(2)-N(2)#5	71.0(4)
O(1)-Gd(1)-O(4)	150.30(16)	O(3)-Gd(2)-O(3)#5	173.3(2)
O(1)-Gd(1)-O(4)#2	88.22(17)	O(6)-Gd(2)-O(3)	63.15(15)
O(3)-Gd(1)-O(6)	68.88(16)	O(6)-Gd(2)-O(3)#5	114.52(15)
O(4)-Gd(1)-O(1)#1	82.93(16)	O(6)#5-Gd(2)-O(3)	114.52(15)
O(4)-Gd(1)-O(4)#2	103.9(2)	O(6)#5-Gd(2)-O(3)#5	63.15(15)
O(4)#2-Gd(1)-O(1)#1	150.23(15)	O(6)-Gd(2)-O(6)#5	143.5(2)
O(7)-Gd(1)-O(1)	86.04(17)	Gd(1)-O(1)-Gd(1)#6	129.45(19)
O(7)-Gd(1)-O(1)#1	83.21(16)	Gd(1)-O(3)-Gd(2)	112.02(18)
O(7)-Gd(1)-O(4)	72.70(14)	Gd(1)-O(4)-Gd(1)#3	103.05(16)
O(7)-Gd(1)-O(4)#2	71.70(14)	Gd(1)-O(6)-Gd(2)	113.25(18)
N(1)-Gd(2)-N(1)#5	152.3(3)	Gd(1)#2-O(7)-Gd(1)	111.76(15)
N(2)-Gd(2)-N(1)	136.3(2)	Gd(1)-O(7)-Gd(1)#3	111.76(15)
N(2)-Gd(2)-N(1)#5	70.5(2)	Gd(1)#2-O(7)-Gd(1)#3	111.76(15)
N(2)#5-Gd(2)-N(1)	70.5(2)		

Symmetry transformations used to generate equivalent atoms: #1: x-y+1,x,-z, #2: -x+y+1,-x+2,z, #3: -y+2,x-y+1,z, #4: x-y+1/3,-y+5/3,-z+1/6, #5: -x+4/3,-x+y+2/3,-z+1/6, #6: y,-x+y+1,-z

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Table S2 Selected Bond Distances (Å) and Bond Angles (deg) for **2.**

bond			
Eu(1)-O(1)	2.405(5)	Eu(2)-O(6)#5	2.483(5)
Eu(1)-O(1)#1	2.555(5)	Eu(2)-O(3)	2.513(5)
Eu(1)-O(3)	2.321(5)	Eu(2)-O(3)#5	2.514(5)
Eu(1)-O(4)	2.433(5)	Eu(2)-N(2)	2.590(7)
Eu(1)-O(4)#2	2.497(5)	Eu(2)-N(2)#5	2.590(7)
Eu(1)-O(6)	2.323(5)	Eu(2)-N(1)	2.670(6)
Eu(1)-O(7)	2.330(2)	O(1)-Eu(1)#6	2.555(5)
Eu(1)-Eu(1)#2	3.8615(5)	O(4)-Eu(1)#3	2.497(5)
Eu(1)-Eu(2)	4.0127(3)	O(7)-Eu(1)#2	2.330(2)
Eu(2)-O(6)	2.482(5)		
angle			
Eu(1)#2-Eu(1)-Eu(1)#3	60	N(2)#5-Eu(2)-N(1)#5	136.1(2)
O(1)-Eu(1)-O(1)#1	74.12(7)	N(2)#5-Eu(2)-N(2)	71.0(4)
O(1)-Eu(1)-O(4)	150.75(16)	O(3)#5-Eu(2)-O(3)	173.7(2)
O(1)-Eu(1)-O(4)#2	88.60(17)	O(6)-Eu(2)-O(3)	63.32(16)
O(3)-Eu(1)-O(6)	68.76(18)	O(6)-Eu(2)-O(3)#5	114.47(16)
O(4)-Eu(1)-O(1)#1	83.17(17)	O(6)#5-Eu(2)-O(3)	114.47(16)
O(4)-Eu(1)-O(4)#2	103.2(2)	O(6)#5-Eu(2)-O(3)#5	63.31(16)
O(4)#2-Eu(1)-O(1)#1	150.33(16)	O(6)#5-Eu(2)-O(6)	143.1(2)
O(7)-Eu(1)-O(1)	86.43(18)	Eu(1)-O(1)-Eu(1)#6	129.13(19)
O(7)-Eu(1)-O(1)#1	83.34(18)	Eu(1)-O(3)-Eu(2)	112.1(2)
O(7)-Eu(1)-O(4)	72.63(15)	Eu(1)-O(4)-Eu(1)#3	103.13(17)
O(7)-Eu(1)-O(4)#2	71.46(15)	Eu(1)-O(6)-Eu(2)	113.13(19)
N(1)#5-Eu(2)-N(1)	152.7(3)	Eu(1)-O(7)-Eu(1)#2	111.89(16)
N(2)-Eu(2)-N(1)	136.1(2)	Eu(1)#3-O(7)-Eu(1)	111.89(16)
N(2)-Eu(2)-N(1)#5	70.3(2)	Eu(1)#3-O(7)-Eu(1)#2	111.89(16)
N(2)#5-Eu(2)-N(1)	70.3(2)		

Symmetry transformations used to generate equivalent atoms: #1: y-1/3,-x+y+1/3,-z+1/3, #2: -y+1,x-y+1,z, #3: -x+y,-x+1,z, #4: -x+1/3,-x+y-1/3,-z+1/6, #5: x-y+1/3,-y+2/3,-z+1/6, #6: x-y+2/3,x+1/3,-z+1/3.

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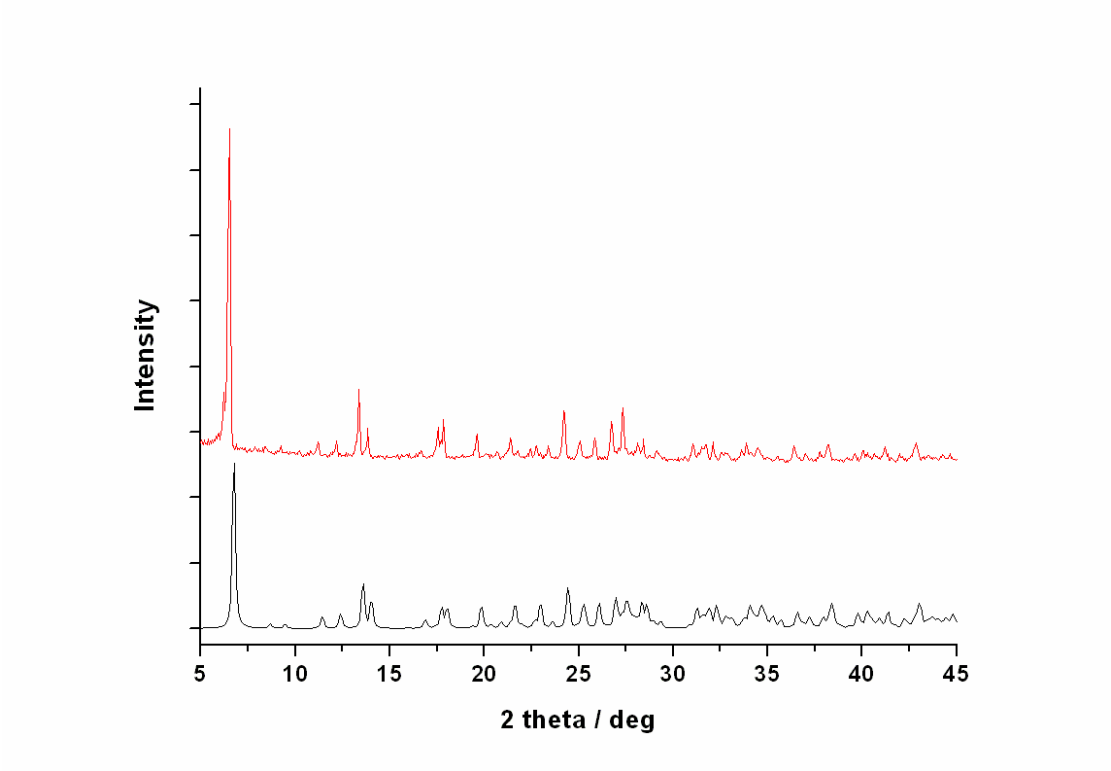
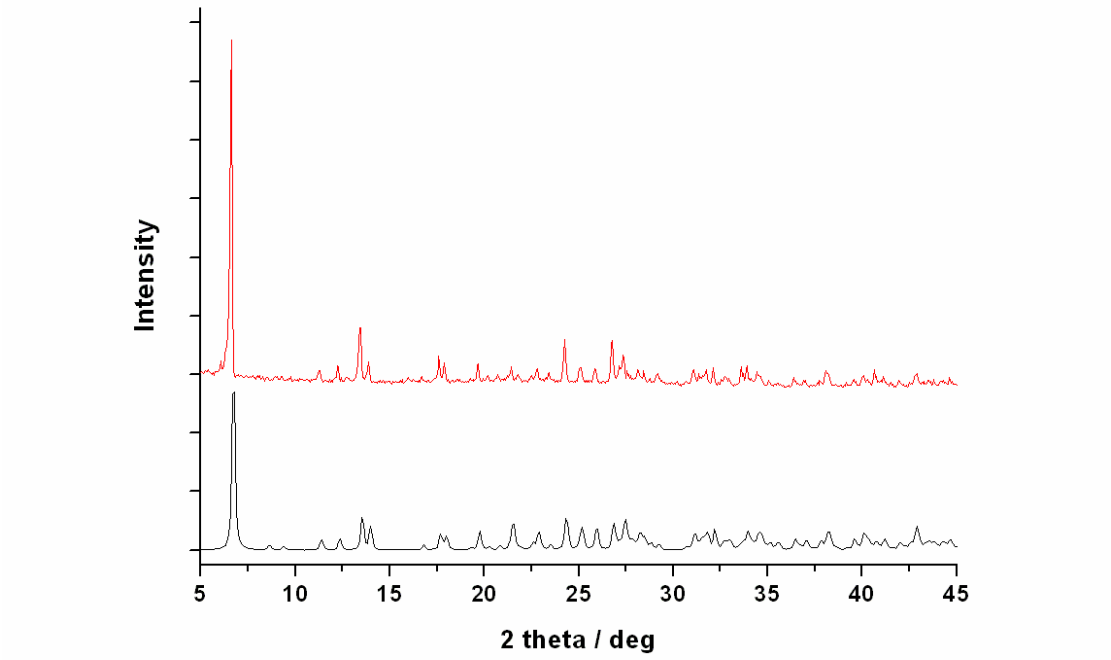


(a)



(b)

Fig. S1 X-ray powder diffraction of complexes **1•Gd** (a) and **2•Eu** (b). Black: simulated from single crystal data; Red: observed for complexes.

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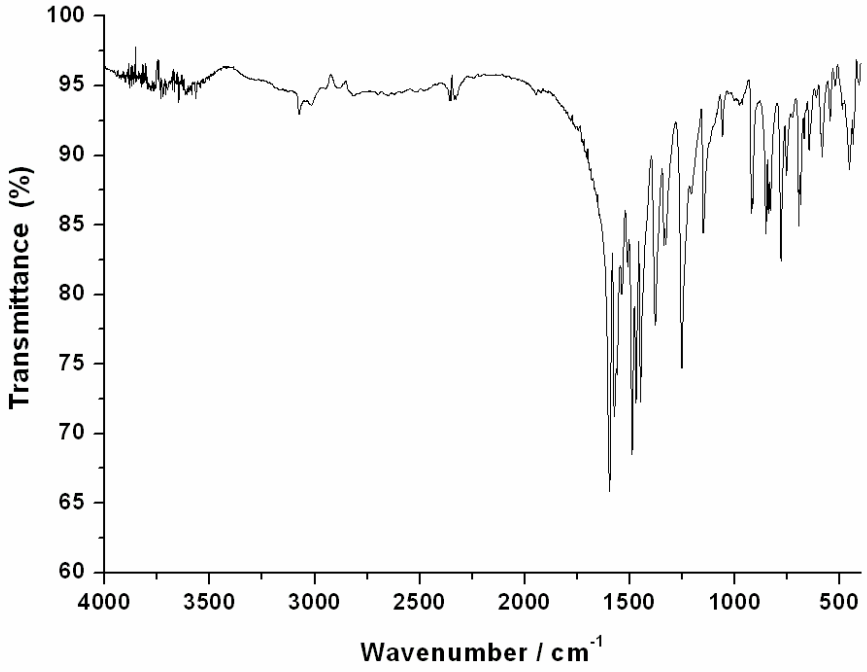
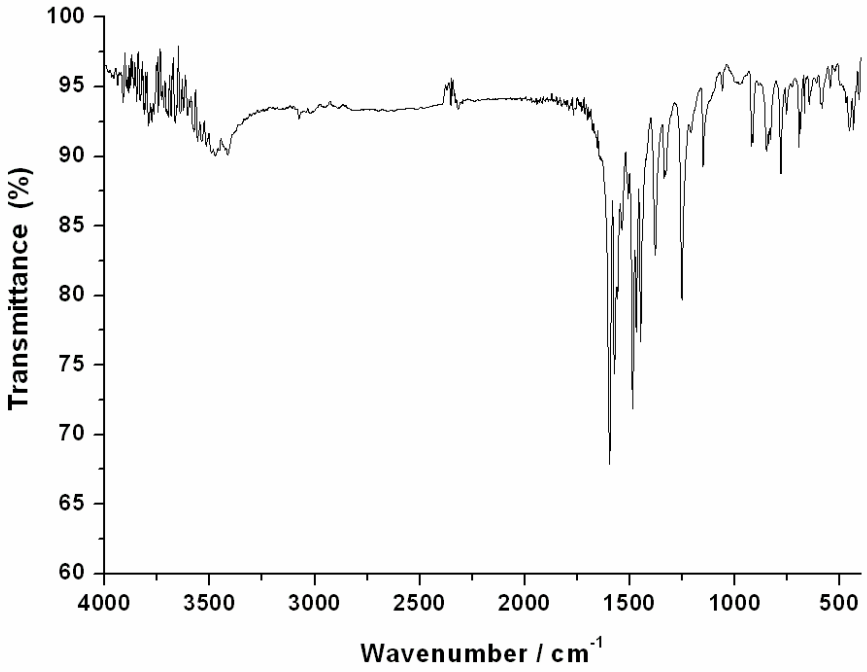


(a)



(b)

Fig. S2 FT-IR spectra for complexes **1•Gd** (a) and **2•Eu** (b).

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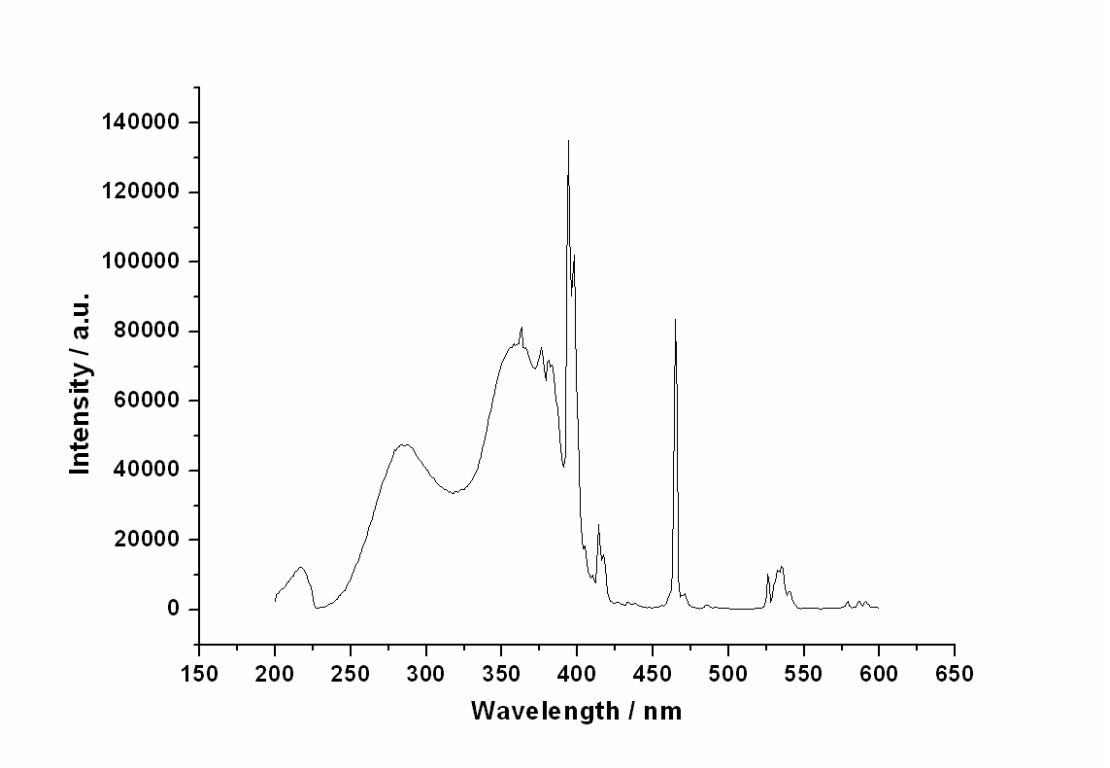

Fig. S3 Solid state excitation spectra of **2•Eu**.