Electronic Supplementary Information (ESI) for

Two Lanthanide Metal–Organic Frameworks Constructed by Tris(4-carboxyphenyl)phosphane Oxide with Gas Adsorption and Magnetic Properties

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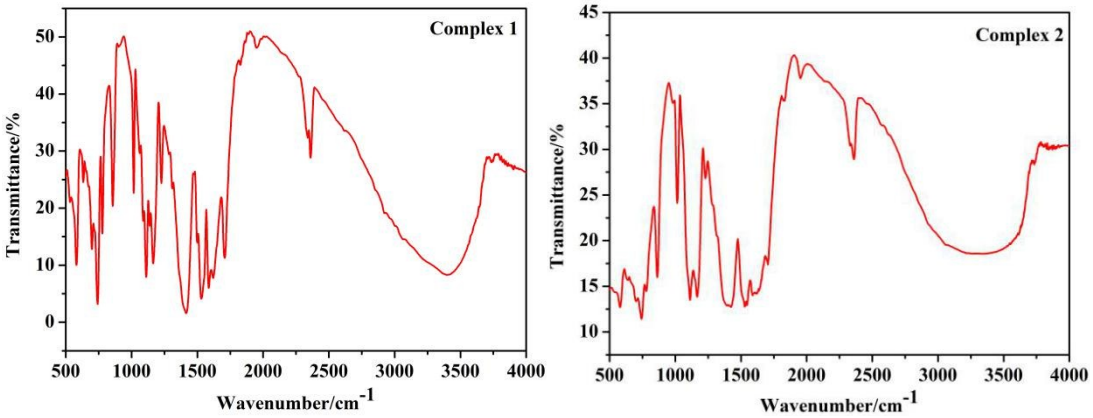

Fig. S1. IR spectra for complexes **1** and **2**.

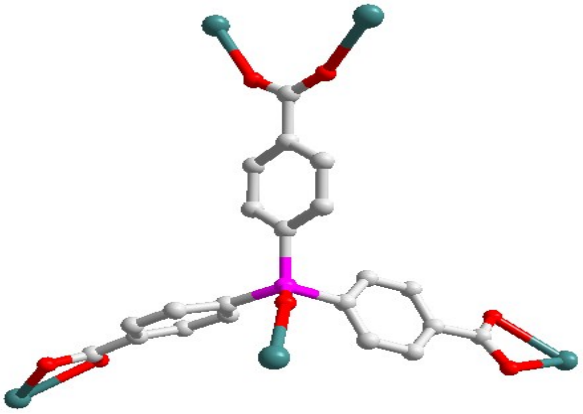

Fig. S2. The coordinated mode of H_3L in **1.**

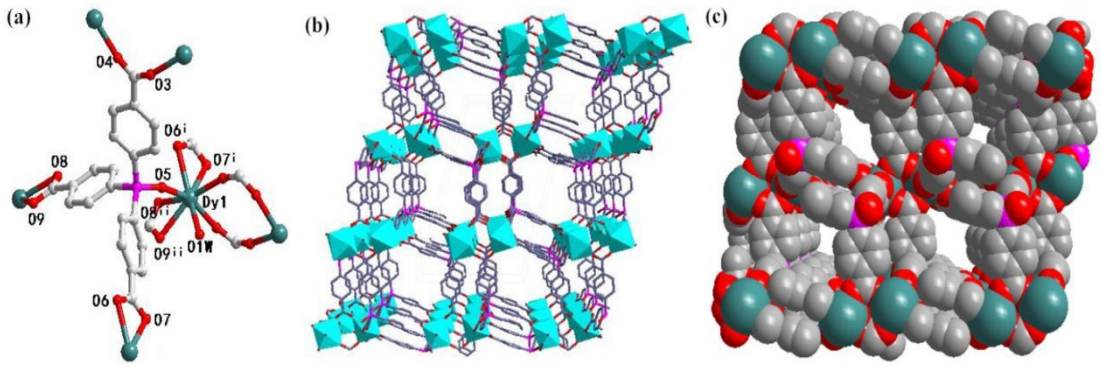

Fig. S3. The coordinated environment of Dy^{III} ion in complex **2.** (Symmetry codes: (*i*) 2-*x*, 1-*y*, 1-*z*; (*ii*) 2-*x*, -*y*, 2-*z*;). (b) Schematic view of the 3D net of **2**. (c) The 3D pack diagram of **2**.

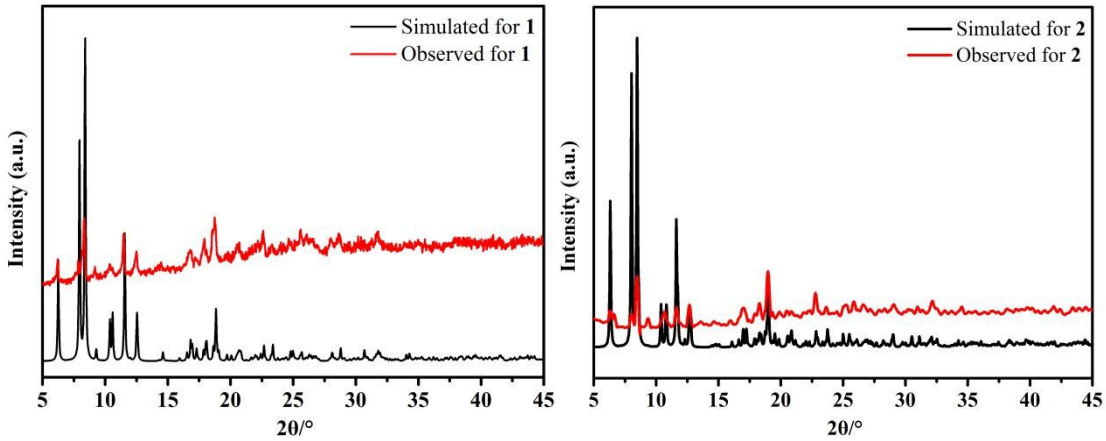

Fig. S4. The PXRD patterns of complexes **1** and **2**.

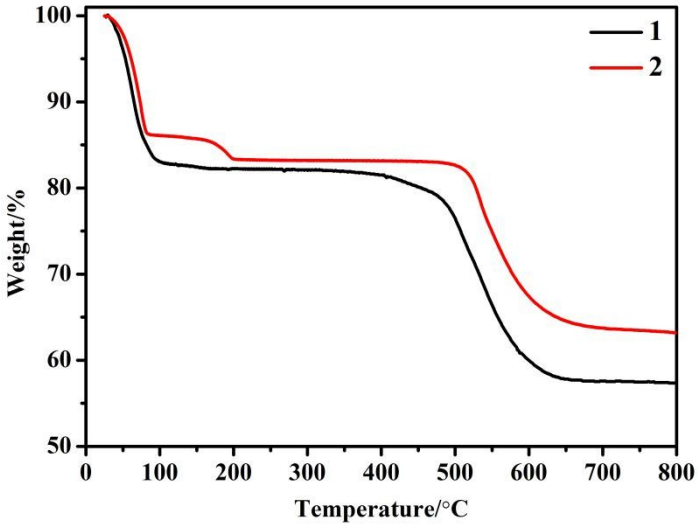

Fig. S5. TGA curves for complexes **1** and **2**.

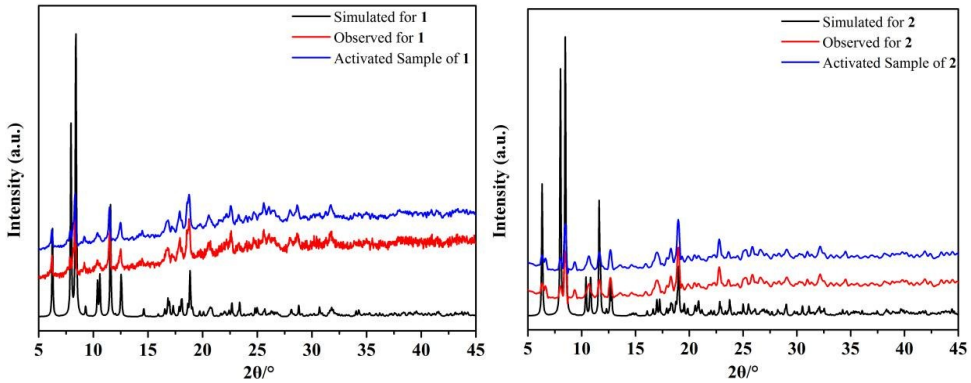

Fig. S6. PXRD patterns of **1** and **2** before and after activating

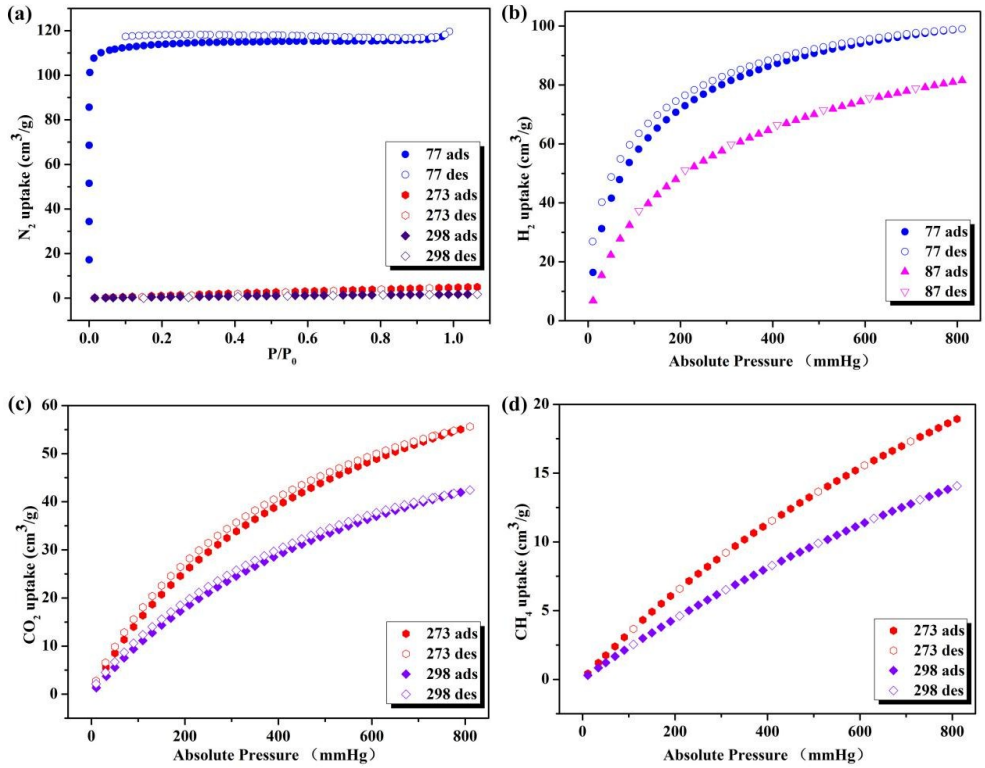

Fig. S7. Gas sorption isotherms of **1**: (a) N_2 at 77 K, 273 K and 298 K; (b) H_2 at 77 K and 87 K; (c) CO_2 at 273 K and 298 K; (d) CH_4 at 273 K and 298 K. ads = adsorption and des =desorption.

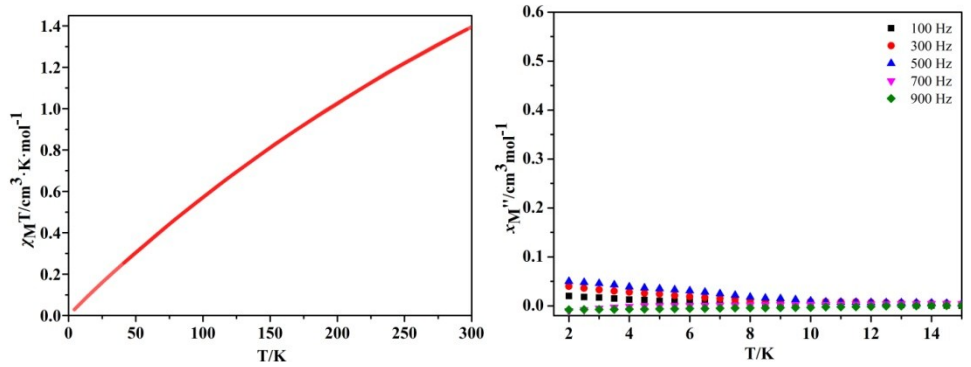

Fig. S8. (a) Temperature-dependent of χMT vs. T with fitting of **1**; (b) Temperature-dependent of the out-of phase (χ''_M) for **1** in a 3.0 AC field oscillating at 100-900 Hz with a zero dc field.

Table S1 Selected bond lengths (Å) and angles (º) for **1** and **2.**

Complex **1**					
Eu(1)-O(2)	2.306(9)	Eu(1)-O(8)^{i}	2.317(8)	Eu(1)-O(1)	2.447(9)
Eu(1)-O(5)^{iii}	2.454(1)	Eu(1)-O(4)^{iii}	2.497(1)	Eu(1)-O(6)^{ii}	2.449(9)
Eu(1)-O(7)^{ii}	2.497(9)	Eu(1)-O(3)^{iv}	2.330(8)		
O(2)-Eu(1)-O(8)^{i}	93.5(3)	O(2)-Eu(1)-O(1)	76.0(3)	O(2)-Eu(1)-O(7)^{ii}	152.5(3)
O(2)-Eu(1)-O(4)^{iii}	81.6(3)	O(2)-Eu(1)-O(6)^{ii}	153.5(4)	O(2)-Eu(1)-O(3)^{iv}	93.2(3)
O(8)^{i}-Eu(1)-O(7)^{ii}	79.1(3)	O(8)^{i}-Eu(1)-O(5)^{iii}	129.5(3)	O(8)^{i}-Eu(1)-O(4)^{iii}	75.9(3)
O(8)^{i}-Eu(1)-O(3)^{iv}	152.1(3)	O(1)-Eu(1)-O(7)^{ii}	76.6(3)	O(1)-Eu(1)-O(5)^{iii}	146.6(3)
O(1)-Eu(1)-O(6)^{ii}	130.3(3)	O(5)^{iii}-Eu(1)-O(7)^{ii}	125.4(3)	O(5)^{iii}-Eu(1)-O(4)^{iii}	53.6(3)
O(6)^{ii}-Eu(1)-O(7)^{ii}	53.9(3)	O(6)^{ii}-Eu(1)-O(5)^{iii}	75.2(4)	O(6)^{ii}-Eu(1)-O(4)^{iii}	77.1(3)
O(3)^{iv}-Eu(1)-O(7)^{ii}	82.5(3)	O(3)^{iv}-Eu(1)-O(5)^{iii}	78.4(3)	O(3)^{iv}-Eu(1)-O(4)^{iii}	131.9(3)
O(2)-Eu(1)-O(5)^{iii}	79.6(3)	O(8)^{i}-Eu(1)-O(1)	76.2(3)	O(8)^{i}-Eu(1)-O(6)^{ii}	96.5(3)
O(1)-Eu(1)-O(4)^{iii}	142.8(3)	O(4)^{iii}-Eu(1)-O(7)^{ii}	121.1(3)	O(3)^{iv}-Eu(1)-O(1)	79.2(3)
O(3)^{iv}-Eu(1)-O(6)^{ii}	89.4(3)				
Symmetry codes: (*i*) 1-*x*, 2-*y*, 1-*z*; (*ii*) 1+*x*, 2-*y*, 1/2+*z*; (*iii*) 1-*x*, 1-*y*, 1-*z*; (*iv*) 1-*x*, +*y*, 3/2-*z*.					
Complex **2**					
Dy(1)-O(1)	2.260(5)	Dy(1)-O(4)	2.282(5)	Dy(1)-O(8)^{i}	2.424(5)
Dy(1)-O(11)^{ii}	2.301(5)	Dy(1)-O(12)^{iii}	2.422(5)	Dy(1)-O(13)^{iii}	2.426(6)
Dy(2)-O(2)	2.288(5)	Dy(2)-O(3)	2.265(5)	Dy(2)-O(5)^{iv}	2.292(5)
Dy(2)-O(7)^{v}	2.410(5)	Dy(2)-O(10)	2.377(6)	Dy(2)-O(14)^{vi}	2.410(5)
Dy(1)-O(9)^{i}	2.410(5)	Dy(1)-O(16)	2.455(6)	Dy(2)-O(6)^{v}	2.437(5)
Dy(2)-O(15)^{vi}	2.418(5)				
O(1)-Dy(1)-O(4)	92.8(0)	O(1)-Dy(1)-O(8)^{i}	157.2(2)	O(1)-Dy(1)-O(9)^{i}	149.0(2)
O(1)-Dy(1)-O(12)^{iii}	80.3(2)	O(1)-Dy(1)-O(13)^{iii}	83.9(2)	O(1)-Dy(1)-O(16)	75.5(2)
O(4)-Dy(1)-O(9)^{i}	82.9(5)	O(4)-Dy(1)-O(11)^{ii}	153.0(8)	O(4)-Dy(1)-O(12)^{iii}	78.2(2)
O(1)-Dy(4)-O(16)	77.6(2)	O(8)^{i}-Dy(1)-O(13)^{iii}	78.8(2)	O(8)^{i}-Dy(1)-O(16)	126.6(2)
O(9)^{i}-Dy(1)-O(12)^{iii}	128.0(6)	O(9)^{i}-Dy(1)-O(13)^{iii}	121.5(2)	O(9)^{i}-Dy(1)-O(16)	73.6(3)
O(11)^{ii}-Dy(1)-O(9)^{i}	81.2(9)	O(11)^{ii}-Dy(1)-O(12)^{iii}	128.5(4)	O(11)^{ii}-Dy(1)-O(13)^{iii}	75.3(4)
O(12)^{iii}-Dy(1)-O(8)^{i}	77.5(0)	O(12)^{iii}-Dy(1)-O(13)^{iii}	53.5(5)	O(12)^{iii}-Dy(1)-O(16)	144.5(9)
O(2)-Dy(2)-O(5)^{iv}	154.6(2)	O(2)-Dy(2)-O(6)^{v}	130.4(2)	O(2)-Dy(2)-O(7)^{v}	76.8(2)
O(2)-Dy(2)-O(14)^{vi}	83.8(2)	O(2)-Dy(2)-O(15)^{vi}	88.2(2)	O(3)-Dy(2)-O(2)	91.6(2)
O(3)-Dy(2)-O(6)^{v}	83.9(2)	O(3)-Dy(2)-O(7)^{v}	80.1(2)	O(3)-Dy(2)-O(10)	76.4(2)
O(3)-Dy(2)-O(15)^{vi}	157.8(2)	O(5)^{iv}-Dy(2)-O(6)^{v}	75.0(7)	O(5)^{iv}-Dy(2)-O(7)^{v}	128.6(6)
O(5)^{iv}-Dy(2)-O(14)^{vi}	80.0(4)	O(5)^{iv}-Dy(2)-O(15)^{vi}	97.6(2)	O(7)^{v}-Dy(2)-O(6)^{v}	53.7(3)
O(7)^{v}-Dy(2)-O(15)^{vi}	78.2(2)	O(10)-Dy(2)-O(6)^{v}	145.0(2)	O(10)-Dy(2)-O(7)^{v}	145.8(2)
O(10)-Dy(2)-O(15)^{vi}	125.2(2)	O(14)^{vi}-Dy(2)-O(6)^{v}	122.2(2)	O(14)^{vi}-Dy(2)-O(15)^{vi}	53.2(9)
O(1)-Dy(1)-O(11)^{ii}	89.6(1)	O(4)-Dy(1)-O(8)^{i}	87.7(2)	O(4)-Dy(1)-O(13)^{iii}	131.6(2)
O(9)^{i}-Dy(1)-O(8)^{i}	53.6(3)	O(11)^{ii}-Dy(1)-O(8)^{i}	100.2(2)	O(11)^{ii}-Dy(1)-O(16)	77.0(9)
O(13)^{iii}-Dy(1)-O(16)	145.5(2)	O(2)-Dy(2)-O(10)	79.4(2)	O(3)-Dy(2)-O(5)^{iv}	92.1(2)
O(3)-Dy(2)-O(14)^{vi}	148.7(2)	O(5)^{iv}-Dy(2)-O(10)	77.0(2)	O(7)^{v}-Dy(2)-O(14)^{vi}	128.1(6)
O(10)-Dy(2)-O(14)^{vi}	72.3(2)	O(15)^{vi}-Dy(2)-O(6)^{v}	79.4(2)		
Symmetry codes: (*i*) 2-*x*, 1-*y*, 1-*z*; (*ii*) 2-*x*, -*y*, 2-*z*; (*iii*) 1-*x*, -*y*, 2-*z*; (*iv*) 2-*x*, -*y*, 1-*z*; (*v*) 1-*x*, -*y*, 1-*z*; (*iv*) 2-*x*, -1-*y*, 2-*z*.					

Table S2 Adsorption uptakes comparisons of complexes **1** and **2** for N_2, H_2, CO_2, CH_4

	N_2			H_2	
	77 K	273 K	298 K	77 K	87 K
Complex **1**	140.7	3.6	2.4	116.5	95.9
Complex **2**	119.6	3.0	2.0	99.0	81.5
	CO_2			CH_4	
	273 K		298 K	273 K	298 K
Complex **1**	65.4		49.9	22.3	16.6
Complex **2**	55.6		42.4	18.9	14.1

Explanation on Alert levels B and C in the cifcheck report

(1) Alert levels B and C in the cifcheck report of complex 1

1) Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.195

Explain: The quality of crystal was not so good with our best effort . So the Rint value was too high. Therefore, the final R1 value was high. Therefore thermal vibration of the atoms was so high that the s.u. of the bonds were high.

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 .....0.195 Report

Explain: The quality of crystal was not so good with our best effort . So the Rint value was too high. Therefore, the final R1 value was high. Therefore thermal vibration of the atoms was so high that the s.u. of the bonds were high.

2) Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check

Explain: The quality of crystal was not so good with our best effort . So the Rint value was too high and ratio of observed reflection was low.

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.4 Note

Explain: The thermal vibration of the atoms was so high, so the atoms with high thermal vibration gave the high ratio of C Ueq(max)/Ueq(min) and U3/U1

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0196 Ang.

Explain: The quality of crystal was not so good with our best effort . So the Rint value was too high. Therefore, the final R1 value was high. Therefore thermal vibration of the atoms was so high that the s.u. of the bonds were high.

(2) Alert levels C in the cifcheck report of complex 2

1) Alert level C

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01121 Ang.

Explain: The quality of crystal was not so good with our best effort . So the Rint value was too high. Therefore, the final R1 value was high. Therefore thermal vibration of the atoms was so high that the s.u. of the bonds were high.