

Supporting Information

Ligand modulated the variable binuclear Cd₂-SBU and structures of four layered coordination frameworks

5

Mengdie Wang,^a Jian Zhang,^a Yunkai Sun,^{*a,c} Jing Wei,^{*b} Chunhong Tan^a and Xiao-Feng Wang^{*a,c}

^a School of Chemistry and Chemical Engineering, University of South China, Hengyang 421001, P. R. China

^b Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, P. R. China.

10 ^c Hunan Province Engineering Research Center of Radioactive Control Technology in Uranium Mining & Metallurgy, University of South China, Hengyang 421001, P. R. China

Email: sunyunkai1983@163.com; weijing@fjirsm.ac.cn; xfwang518@sina.cn.

Table S1. Crystallographic data for complexes **1-4**.

Compound	1	2	3	4
Formula	C ₃₂ H ₂₀ Cd ₂ N ₄ O ₈	C ₄₆ H ₃₈ Cd ₂ N ₆ O ₁₀	C ₄₈ H ₂₉ Cd ₂ N ₄ O _{8.50}	C ₅₀ H ₄₂ Cd ₂ N ₆ O ₁₀
Mr	813.34	1059.62	1022.55	1111.69
Temp (K)	296	173	200	296
Cryst system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>C</i> 2/ <i>c</i>
<i>a</i> /Å	11.2212(14)	11.9395(9)	11.4363(4)	15.7433(4)
<i>b</i> /Å	20.067(3)	19.2586(14)	14.5488(3)	16.0405(4)
<i>c</i> /Å	13.8260(17)	18.4785(13)	11.9096(3)	20.0977(5)
α /°	90	90	90	90
β /°	107.713(4)	98.580(2)	94.848(3)	102.843(10)
γ /°	90	90	90	90
<i>V</i> /Å ³	2965.7(7)	4201.4(5)	1974.48(9)	4948.3(2)
<i>Z</i>	4	4	2	4
<i>D</i> _c /g cm ⁻³	1.822	1.675	1.720	1.492
μ /mm ⁻¹	1.494	1.081	9.178	0.922
<i>F</i> (000)	1600	2128	1018	2240
<i>R</i> (int)	0.0269	0.0432	0.0508	0.0385
Total reflections	63576	139946	22097	55538
Unique reflections	6826	9712	3904	5712
<i>I</i> > 2σ(<i>I</i>)	6213	8196	3411	5117
<i>R</i> ₁	0.0334	0.0296	0.0254	0.0375
<i>wR</i> ₂	0.1111	0.1115	0.0608	0.1174
<i>S</i>	1.06	1.18	1.04	1.13

Table S2. Selected bond distances (Å) for complexes **1-4**.

1		2		3		4	
Cd1-O1	2.307(19)	Cd1-O1	2.495(19)	Cd1-O1	2.433(19)	Cd1-O2	2.280(2)
Cd1-O3	2.365(2)	Cd1-O2	2.282(18)	Cd1-O2	2.338(18)	Cd1-N1	2.383(3)
Cd1-O4	2.330(2)	Cd1-O3	2.423(19)	Cd1-N1	2.348(2)	Cd1-N2	2.367(3)
Cd1-O6	2.390(2)	Cd1-O4	2.511(2)	Cd1-N2	2.345(2)	Cd1-O1a	2.285(2)
Cd1-N1	2.340(2)	Cd1-O5	2.299(19)	Cd1-O3a	2.459(2)	Cd1-O4a	2.261(2)
Cd1-N2	2.362(2)	Cd1-N1	2.348(2)	Cd1-O4a	2.407(2)	Cd1-O3	2.291(3)
Cd2-O1	2.299(2)	Cd1-N2	2.352(2)	Cd1-O3	2.314(18)		
Cd2-O5	2.253(2)	Cd2-O4	2.288(2)				
Cd2-O7	2.238(7)	Cd2-O6	2.302(18)				
Cd2-O8	2.465(7)	Cd2-O7	2.337(2)				
Cd2-N3	2.346(2)	Cd2-O8	2.432(2)				
Cd2-N4	2.322(2)	Cd2-N3	2.337(2)				
Cd2-O7'	2.287(3)	Cd2-N4	2.352(2)				
Cd2-O8'	2.475(4)						

Table S3. Selected bond angles (°) for complexes **1-4**.

1		2		3		4	
O1-Cd1-O3	154.68(9)	O1-Cd1-O2	54.48(6)	O1-Cd1-O2	55.06(6)	O2-Cd1-N1	125.40(10)
O1-Cd1-O4	103.86(8)	O1-Cd1-O3	132.57(7)	O1-Cd1-N1	92.44(7)	O2-Cd1-N2	84.67(10)
O1-Cd1-N1	106.22(8)	O1-Cd1-O4	173.16(6)	O1-Cd1-N2	156.27(7)	O1a-Cd1-O2	83.16(10)
O1-Cd1-N2	94.63(7)	O1-Cd1-O5	96.12(7)	O1-Cd1-O3a	82.60(6)	O2-Cd1-O4a	148.65(9)
O3-Cd1-O4	55.41(8)	O1-Cd1-N1	89.42(7)	O1-Cd1-O4a	122.74(6)	O2-Cd1-O3	83.68(10)
O3-Cd1-N1	98.75(9)	O1-Cd1-N2	82.86(6)	O1-Cd1-O3	82.11(6)	N1-Cd1-N2	68.58(12)
O3-Cd1-N2	89.51(9)	O2-Cd1-O3	82.11(7)	O2-Cd1-N1	91.31(7)	O1a-Cd1-N1	79.76(10)
O4-Cd1-N1	142.70(8)	O2-Cd1-O4	127.84(6)	O2-Cd1-N2	139.23(7)	O4a-Cd1-N1	82.81(10)
O4-Cd1-N2	127.92(8)	O2-Cd1-O5	101.09(7)	O2-Cd1-O3a	82.36(6)	O3-Cd1-N1	134.75(11)
O1-Cd1-O6	81.53(7)	O2-Cd1-N1	103.95(8)	O2-Cd1-O4a	81.30(7)	O1a-Cd1-N2	129.77(10)
O4-Cd1-O6	80.68(8)	O2-Cd1-N2	137.32(7)	O2-Cd1-O3	134.53(7)	O4a-Cd1-N2	121.99(10)
N1-Cd1-O6	82.43(7)	O3-Cd1-O4	52.81(6)	N1-Cd1-N2	71.16(8)	O3-Cd1-N2	82.77(10)
N2-Cd1-O6	150.87(7)	O3-Cd1-O5	111.68(7)	O3a-Cd1-N1	173.46(7)	O1a-Cd1-O4a	89.89(10)
O3-Cd1-O6	106.28(8)	O3-Cd1-N1	82.94(8)	O4a-Cd1-N1	126.94(8)	O1a-Cd1-O3	143.18(10)
N1-Cd1-N2	70.87(8)	O3-Cd1-N2	136.26(7)	O3-Cd1-N1	106.44(7)	O3-Cd1-O4a	83.86(10)
O5-Cd2-O1	92.34(3)	O4-Cd1-O5	77.21(7)	O3a-Cd1-N2	114.84(7)		
O5-Cd2-O7	121.9(3)	O4-Cd1-N1	95.83(7)	O4a-Cd1-N2	80.96(7)		
O5-Cd2-O8	80.12(19)	O4-Cd1-N2	94.66(6)	O3-Cd1-N2	86.20(7)		
O5-Cd2-N3	142.14(7)	O5-Cd1-N1	152.56(7)				
O5-Cd2-N4	92.97(9)	O5-Cd1-N2	82.92(6)				
O1-Cd2-O7	94.3(3)	N1-Cd1-N2	71.10(7)				
O1-Cd2-O8	133.4(3)	O4-Cd2-O6	100.21(8)				
O1-Cd2-N3	80.14(19)	O4-Cd2-N3	84.79(7)				

O1-Cd2-N4	144.54(7)	O4-Cd2-N4	152.48(7)	
O7-Cd2-O8	54.8(3)	O4-Cd2-O7	110.57(8)	
O7-Cd2-N3	96.0(3)	O4-Cd2-O8	98.07(7)	
O7-Cd2-N4	112.2(3)	N3-Cd2-N4	71.44(7)	
O8-Cd2-N3	128.8(3)	O7-Cd2-N3	136.66(7)	
O8-Cd2-N4	82.0(3)	O8-Cd2-N3	84.12(7)	
N3-Cd2-N4	71.44(7)	O7-Cd2-N4	96.42(9)	
O5-Cd2-O7'	81.17(10)	O8-Cd2-N4	93.20(8)	
O1-Cd2-O7'	102.55(16)	O7-Cd2-O8	54.42(7)	
N3-Cd2-O7'	136.70(10)			
N4-Cd2-O7'	112.86(16)			
O5-Cd2-O8'	130.39(10)			
O1-Cd2-O8'	113.05(17)			
O7'-Cd2-O8'	52.90(11)			
N3-Cd2-O8'	85.06(9)			
N4-Cd2-O8'	89.41(17)			

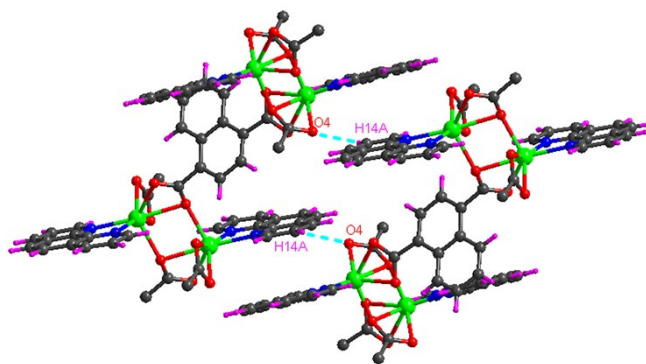


Figure S1. H-bonds between adjacent layers in **3**

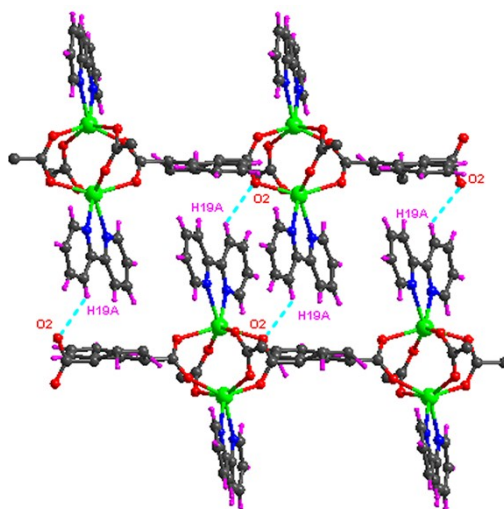


Figure S2. H-bonds between adjacent layers in **4**

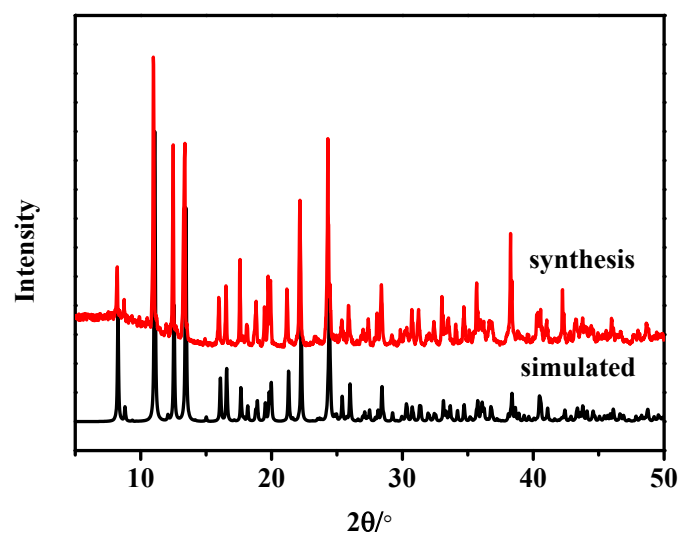


Figure S3. The PXRD curve of **1**

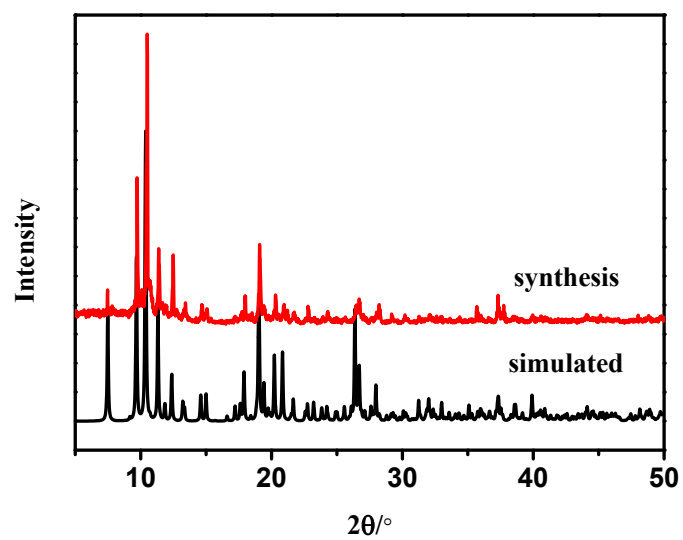


Figure S4. The PXRD curve of **2**

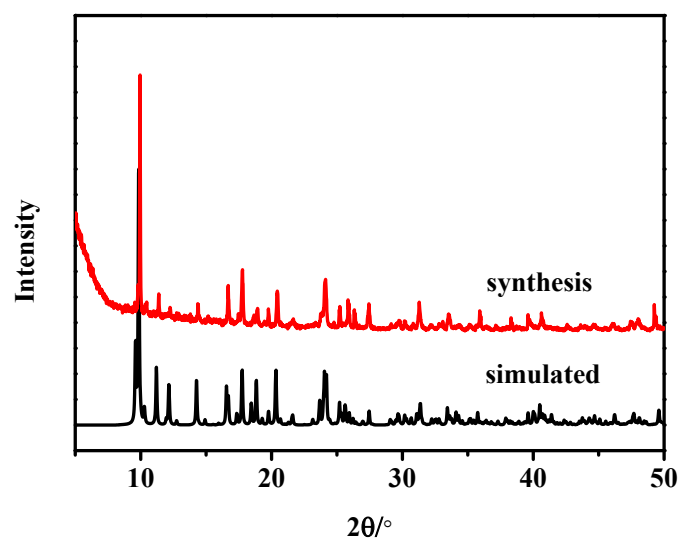


Figure S5. The PXRD curve of **3**

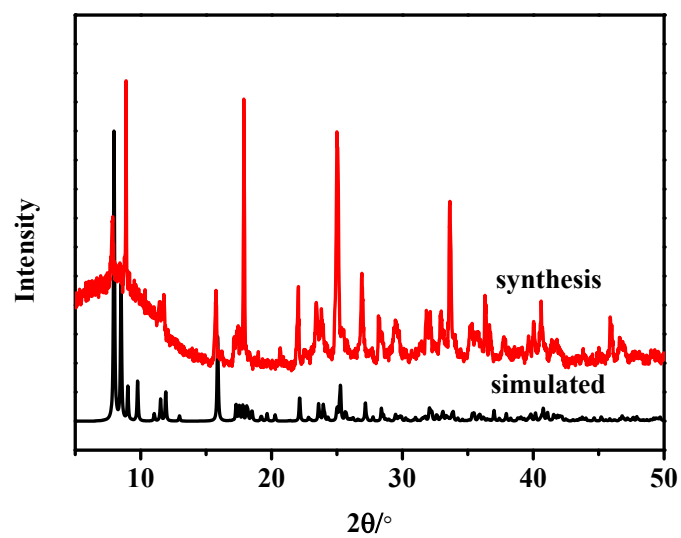


Figure S6. The PXRD curve of **4**

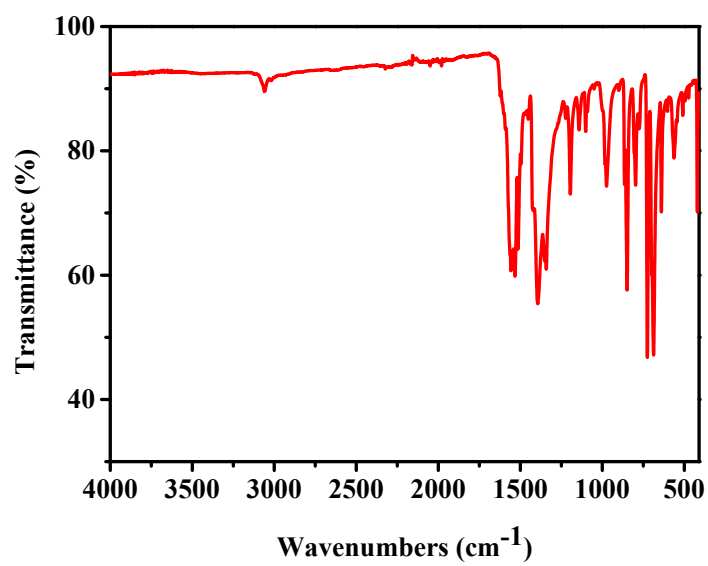


Figure S7. The FT-IR pattern of **1**

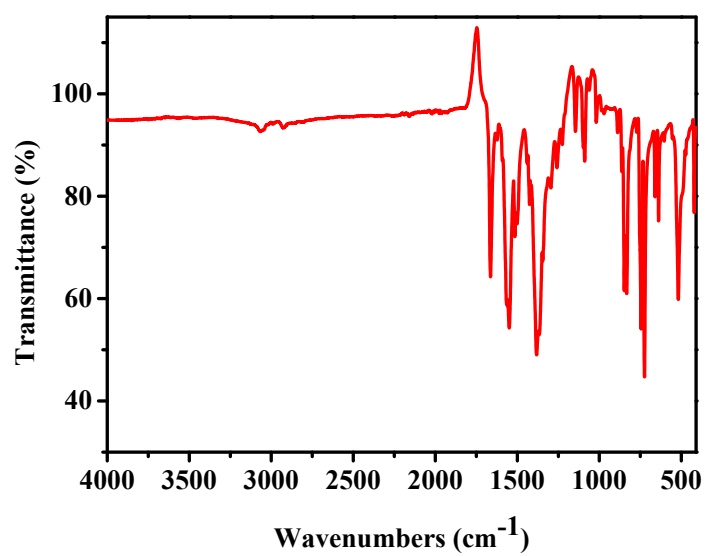


Figure S8. The FT-IR pattern of 2

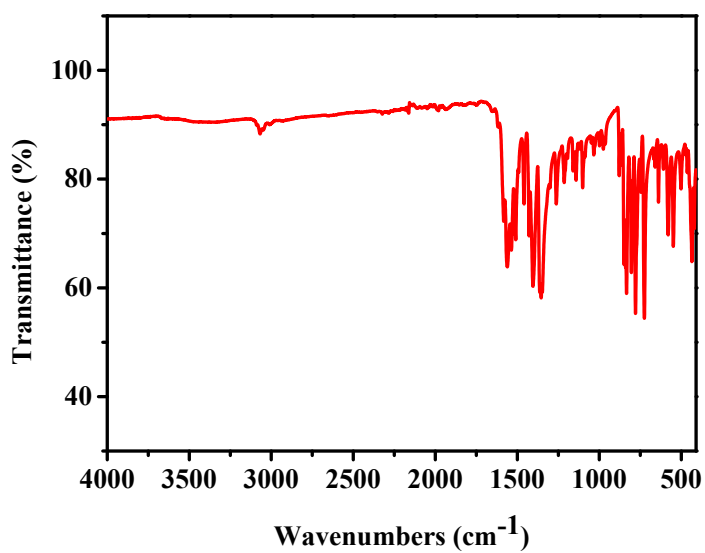


Figure S9. The FT-IR pattern of 3

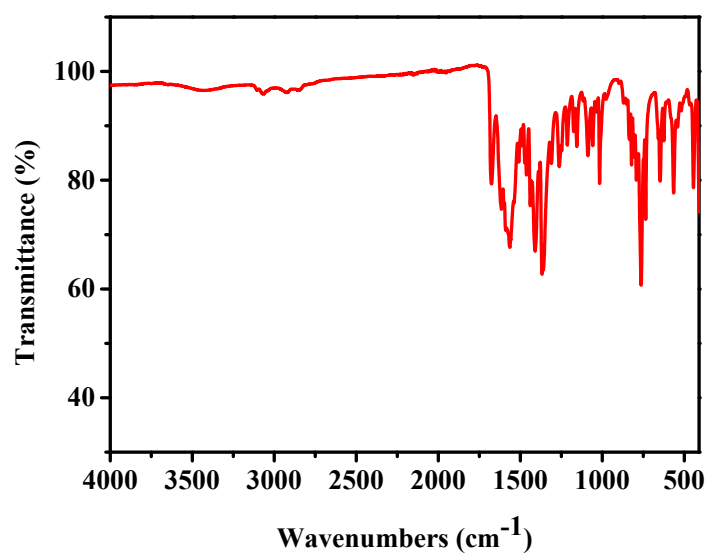


Figure S10. The FT-IR pattern of **4**

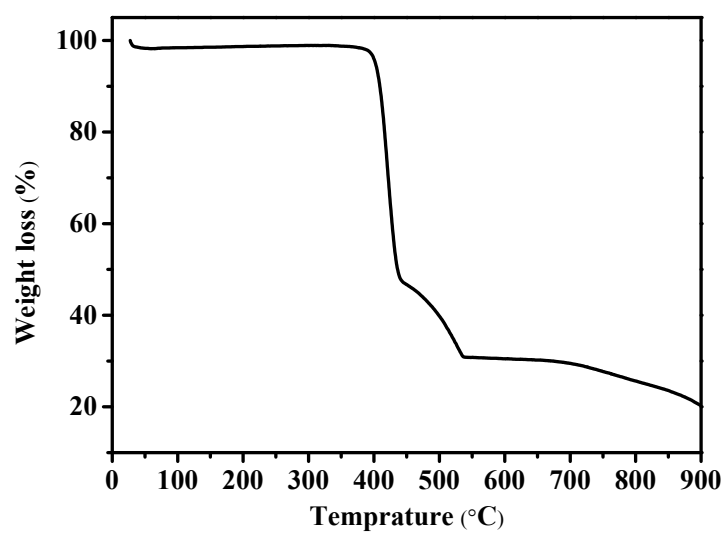


Figure S11. The TGA curve of **1**

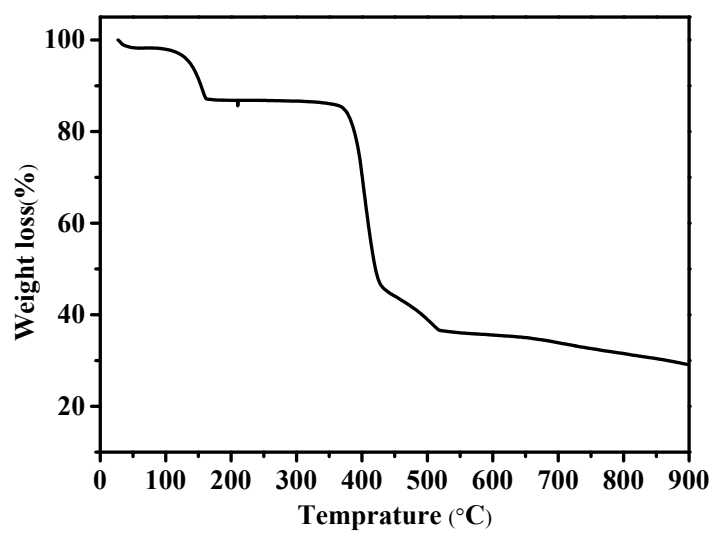


Figure S12. The TGA curve of **2**

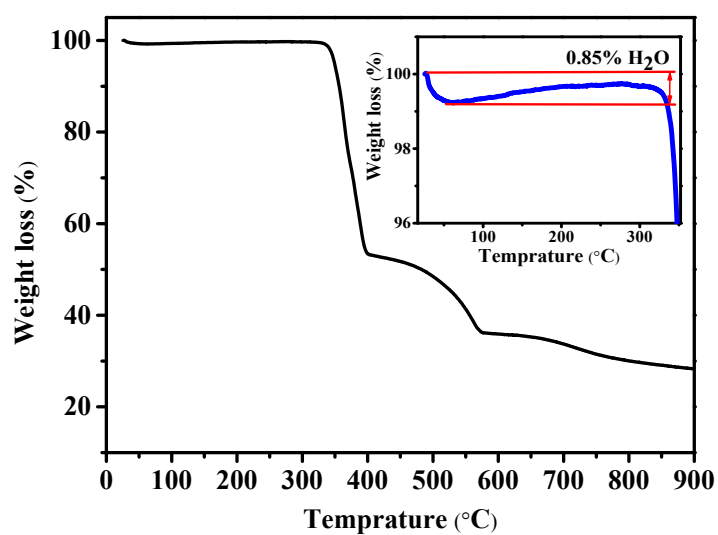


Figure S13. The TGA curve of **3**

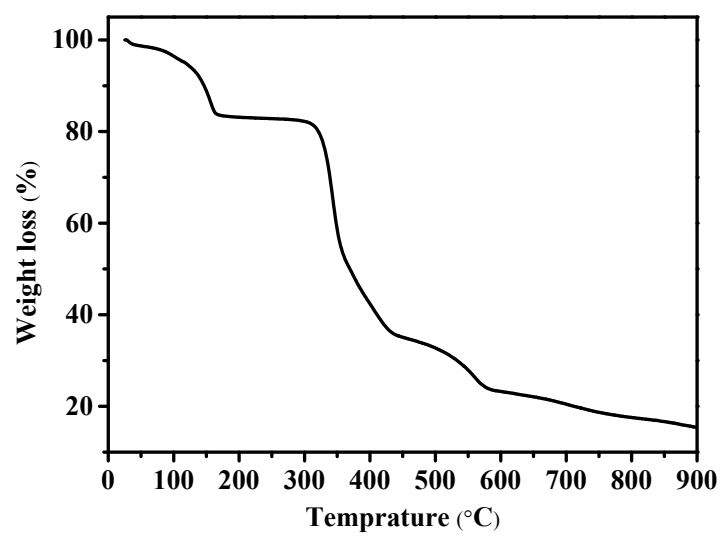


Figure S14. The TGA curve of **4**