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A family of Uranium-carboxylic acid hybrid materials: synthesis, structure and mixed-dyes selective adsorption

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Table S1 Selected bond distances (Å) and angles (°) of complexes **1-4***

Complex **1**			
U(1)-O(1)	1.755(3)	U(1)-O(2)	1.770(3)
U(1)-O(5)	2.355(2)	U(1)-O(6)	2.363(2)
U(1)-O(7)$^{\#1}$	2.364(3)	U(1)-O(3)	2.393(2)
U(1)-O(4)	2.408(3)		
O(1)-U(1)-O(2)	179.15(13)	O(1)-U(1)-O(5)	87.95(11)
O(2)-U(1)-O(5)	91.67(11)	O(1)-U(1)-O(6)	95.35(10)
O(2)-U(1)-O(6)	85.21(10)	O(5)-U(1)-O(6)	67.76(8)
O(1)-U(1)-O(7)$^{\#1}$	86.64(11)	O(2)-U(1)-O(7)$^{\#1}$	94.12(11)
O(5)-U(1)-O(7)$^{\#1}$	142.52(9)	O(6)-U(1)-O(7)$^{\#1}$	75.87(9)
O(1)-U(1)-O(3)	93.35(11)	O(2)-U(1)-O(3)	86.49(11)
O(5)-U(1)-O(3)	142.83(9)	O(6)-U(1)-O(3)	148.56(9)
O(7)$^{\#1}$-U(1)-O(3)	74.55(9)	O(1)-U(1)-O(4)	89.41(12)
O(2)-U(1)-O(4)	89.75(12)	O(5)-U(1)-O(4)	71.24(9)
O(6)-U(1)-O(4)	138.49(9)	O(7)$^{\#1}$-U(1)-O(4)	145.64(9)
O(3)-U(1)-O(4)	71.63(9)		
Complex **2**			
U(1)-O(1)	1.775(3)	U(1)-O(1)$^{\#1}$	1.775(3)
U(1)-O(2)	2.452(3)	U(1)-O(2)$^{\#1}$	2.452(2)
U(1)-O(4)	2.472(3)	U(1)-O(4)$^{\#1}$	2.472(3)
U(1)-O(3)	2.503(3)	U(1)-O(3)$^{\#1}$	2.503(3)
O(1)-U(1)-O(1)$^{\#1}$	179.999(1)	O(1)-U(1)-O(2)	92.80(13)
O(1)-U(1)-O(2)$^{\#1}$	87.20(13)	O(1)$^{\#1}$-U(1)-O(2)	87.20(13)
O(1)$^{\#1}$-U(1)-O(2)$^{\#1}$	92.80(13)	O(2)-U(1)-O(2)$^{\#1}$	180.0
O(1)#1-U(1)-O(4)$^{\#1}$	93.60(13)	O(1)-U(1)-O(4)$^{\#1}$	86.40(13)
O(2)-U(1)-O(4)$^{\#1}$	62.80(10)	O(2)$^{\#1}$-U(1)-O(4)$^{\#1}$	117.20(10)
O(1)$^{\#1}$-U(1)-O(4)	86.40(13)	O(1)-U(1)-O(4)	93.60(13)
O(2)-U(1)-O(4)	117.20(10)	O(2)$^{\#1}$-U(1)-O(4)	62.80(10)
O(4)-U(1)-O(4)$^{\#1}$	180.0	O(1)$^{\#1}$-U(1)-O(3)$^{\#1}$	87.77(13)
O(1)-U(1)-O(3)$^{\#1}$	92.23(13)	O(2)-U(1)-O(3)$^{\#1}$	114.15(10)

$O(2)^{\#1}$-U(1)-$O(3)^{\#1}$	65.85(10)	$O(4)^{\#1}$-U(1)-$O(3)^{\#1}$	52.12(10)
O(4)-U(1)-$O(3)^{\#1}$	127.88(10)	$O(1)^{\#1}$-U(1)-O(3)	92.23(13)
O(1)-U(1)-O(3)	87.76(13)	O(2)-U(1)-O(3)	65.85(10)
$O(2)^{\#1}$-U(1)-O(3)	114.15(10)	$O(4)^{\#1}$-U(1)-O(3)	127.88(10)
O(4)-U(1)-O(3)	52.12(10)	O(3)-U(1)-$O(3)^{\#1}$	180.0
Complex **3**			
U(1)-O(1)	1.755(4)	U(1)-O(2)	1.763(4)
U(1)-O(8)	2.392(5)	U(1)-O(3)	2.436(5)
U(1)-O(4)	2.464(4)	U(1)-O(5)	2.477(4)
U(1)-O(7)	2.493(5)	U(1)-O(6)	2.494(5)
O(1)-U(1)-O(2)	178.3(2)	O(1)-U(1)-O(8)	92.4(2)
O(2)-U(1)-O(8)	88.7(2)	O(1)-U(1)-O(3)	90.8(2)
O(2)-U(1)-O(3)	90.9(2)	O(8)-U(1)-O(3)	67.9(2)
O(1)-U(1)-O(4)	91.5(2)	O(2)-U(1)-O(4)	89.1(2)
O(8)-U(1)-O(4)	121.2(2)	O(3)-U(1)-O(4)	53.4(2)
O(1)-U(1)-O(5)	90.4(2)	O(2)-U(1)-O(5)	88.4(2)
O(8)-U(1)-O(5)	172.4(2)	O(3)-U(1)-O(5)	119.2(2)
O(4)-U(1)-O(5)	65.8(2)	O(1)-U(1)-O(7)	89.5(2)
O(2)-U(1)-O(7)	90.1(2)	O(8)-U(1)-O(7)	52.8(2)
O(3)-U(1)-O(7)	120.7(2)	O(4)-U(1)-O(7)	174.0(2)
O(5)-U(1)-O(7)	120.1(2)	O(1)-U(1)-O(6)	88.2(2)
O(2)-U(1)-O(6)	90.1(2)	O(8)-U(1)-O(6)	121.0(2)
O(3)-U(1)-O(6)	171.1(2)	O(4)-U(1)-O(6)	117.8(2)
O(5)-U(1)-O(6)	52.0(1)	O(7)-U(1)-O(6)	68.2(2)
Complex **4**			
U(1)-O(1)	1.768(5)	U(1)-O(2)	1.772(5)
U(1)-O(6)	2.289(5)	U(1)-O(5)	2.306(5)
U(1)-O(8)	2.460(5)	U(1)-O(12)	2.482(5)
U(1)-O(7)	2.487(5)	U(2)-O(4)	1.762(5)
U(2)-O(3)	1.769(5)	$U(2)-O(5)^{\#1}$	2.296(5)
$U(2)-O(6)^{\#2}$	2.308(5)	U(2)-O(9)	2.468(5)

U(2)-O(11)	2.479(5)	U(2)-O(10)	2.487(5)
O(1)-U(1)-O(2)	178.1(2)	O(1)-U(1)-O(6)	86.9(2)
O(2)-U(1)-O(6)	92.9(2)	O(1)-U(1)-O(5)	94.9(2)
O(2)-U(1)-O(5)	87.0(2)	O(6)-U(1)-O(5)	83.50(17)
O(1)-U(1)-O(8)	89.9(2)	O(2)-U(1)-O(8)	89.1(2)
O(6)-U(1)-O(8)	142.53(17)	O(5)-U(1)-O(8)	133.96(16)
O(1)-U(1)-O(12)	94.6(2)	O(2)-U(1)-O(12)	83.6(2)
O(6)-U(1)-O(12)	74.64(17)	O(5)-U(1)-O(12)	155.62(17)
O(8)-U(1)-O(12)	68.43(16)	O(1)-U(1)-O(7)	86.9(2)
O(2)-U(1)-O(7)	94.1(2)	O(6)-U(1)-O(7)	152.03(17)
O(5)-U(1)-O(7)	69.91(16)	O(8)-U(1)-O(7)	64.66(15)
O(12)-U(1)-O(7)	133.06(16)	O(4)-U(2)-O(3)	179.7(2)
O(4)-U(2)-O(5)$^{\#1}$	89.1(2)	O(3)-U(2)-O(5)$^{\#1}$	90.7(2)
O(4)-U(2)-O(6)$^{\#2}$	90.5(2)	O(3)-U(2)-O(6)$^{\#2}$	89.7(2)
O(5)$^{\#1}$-U(2)-O(6)$^{\#2}$	81.39(17)	O(4)-U(2)-O(9)	87.7(2)
O(3)-U(2)-O(9)	92.6(2)	O(5)$^{\#1}$-U(2)-O(9)	154.44(16)
O(6)$^{\#2}$-U(2)-O(9)	73.29(17)	O(4)-U(2)-O(11)	85.9(2)
O(3)-U(2)-O(11)	93.8(2)	O(5)$^{\#1}$-U(2)-O(11)	73.09(16)
O(6)$^{\#2}$-U(2)-O(11)	154.27(17)	O(9)-U(2)-O(11)	131.86(16)
O(4)-U(2)-O(10)	91.3(2)	O(3)-U(2)-O(10)	88.8(2)
O(5)$^{\#1}$-U(2)-O(10)	140.18(16)	O(6)$^{\#2}$-U(2)-O(10)	138.41(17)
O(9)-U(2)-O(10)	65.28(15)	O(11)-U(2)-O(10)	67.22(16)

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

Table S2 Hydrogen bond lengths (Å) and angles (°) for complexes **1-4***

D-H···A	d-D(H)/Å	d(H···A)/Å	d(D···A)/Å	∠D–H···A/°
Complex **1**				
O(4)-H(4B)···O(9)	0.85	1.82	2.530(4)	139.2
N(1)-H(1)···O(8)$^{\#2}$	0.86	1.87	2.686(4)	157.2
O(4)-H(4A)...O(8)$^{\#3}$	0.85	1.93	2.682(4)	146.0
C(12)-H(12)···O(2)$^{\#4}$	0.93	2.58	3.347(5)	139.8
Complex **2**				
O(2)-H(2A)···O(1)$^{\#2}$	0.85	2.50	3.028(4)	120.9
Complex **3**				
N(1)-H(1A)···O(5)	0.90	1.87	2.757(7)	166.3
N(1)-H(1B)···O(2)$^{\#1}$	0.90	2.11	2.915(7)	148.8
Complex **4**				
O(1W)-H(1WB)···O(8)	0.85	1.97	2.818(9)	175.2
O(1W)-H(1WA)···O(12)$^{\#5}$	0.85	2.30	3.144(11)	173.7
O(12)-H(12A)···O(9)$^{\#4}$	0.85	1.95	2.769(7)	161.0

*Symmetry transformation used to generate equivalent atoms: complex **1**: #2: -x+1, -y, -z, #3: -x+3/2, y+1/2, -z+1/2, #4: x-1/2, -y-1/2, z-1/2; complex **2**: #2: -x, -y+1, -z+1; complex **3**: #1: x, -y+1/2, z+1/2; complex **4**: #4: -x+1, y+1/2, -z+3/2, #5: x+1, y, z.

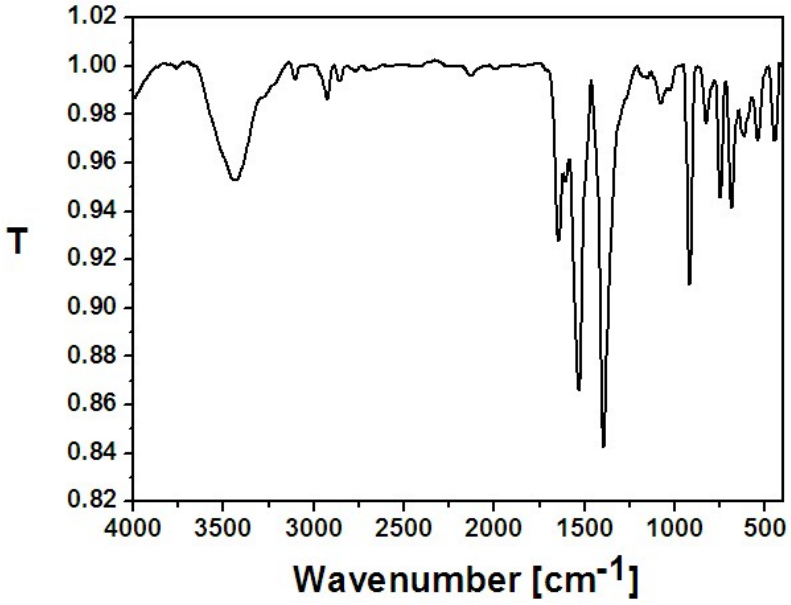

Fig. S1 The Solid-state IR spectra of complex **1** at a room temperature.

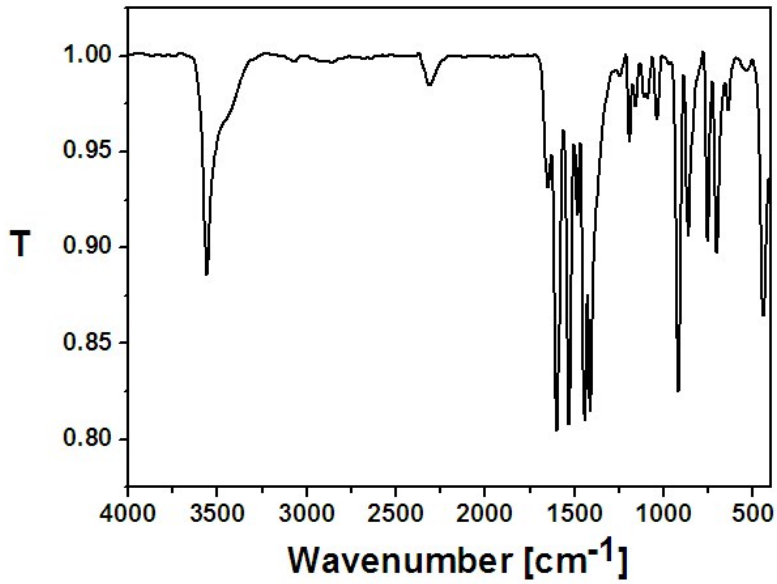

Fig. S2 The Solid-state IR spectra of complex **2** at a room temperature.

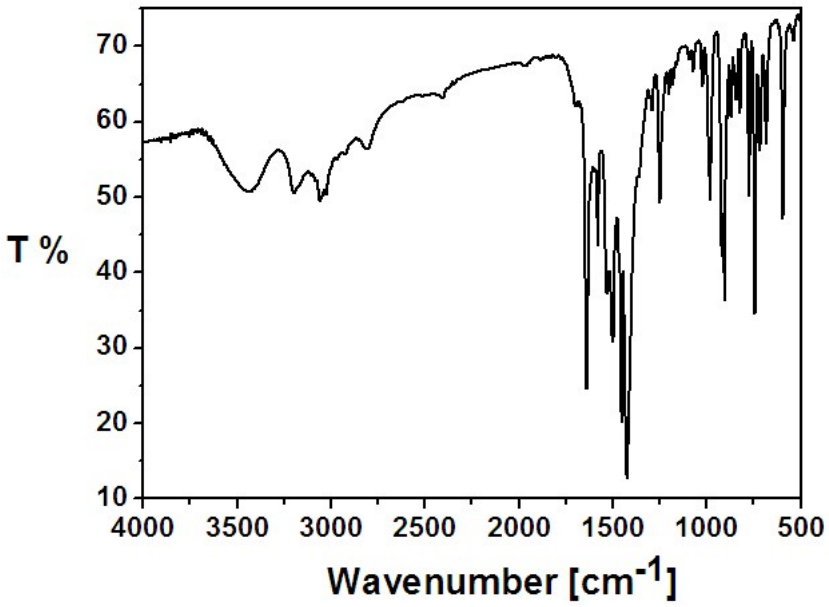

Fig. S3 The Solid-state IR spectra of complex **3** at a room temperature.

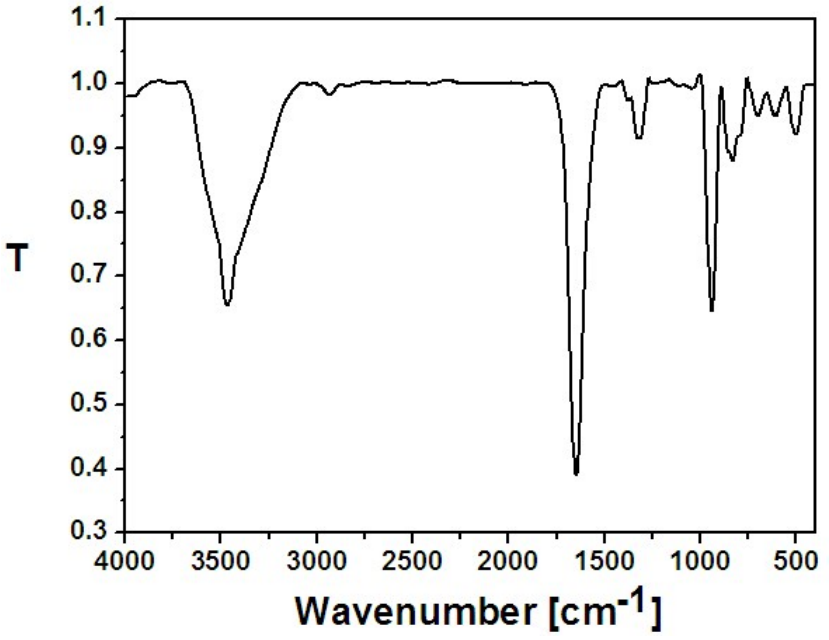

Fig. S4 The Solid-state IR spectra of complex **4** at a room temperature.

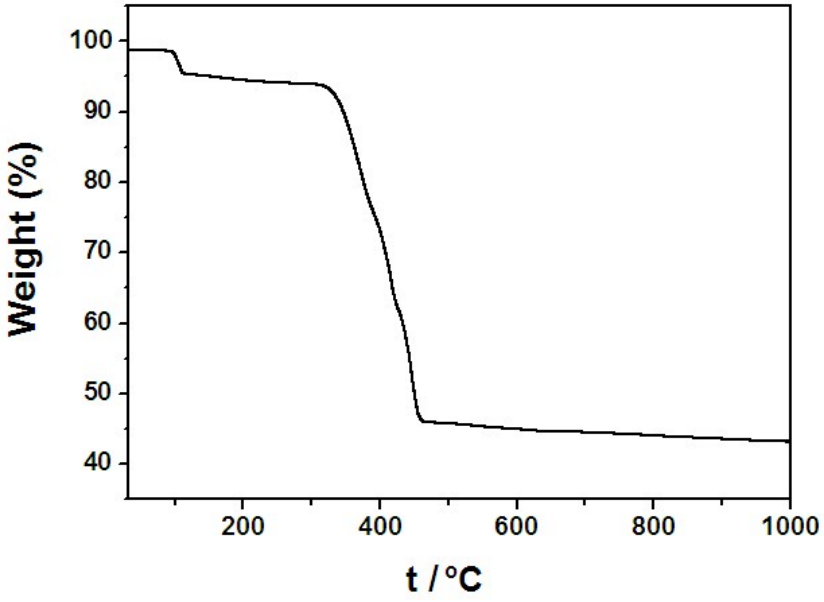

Fig. S5 The TG curve for complex **1**.

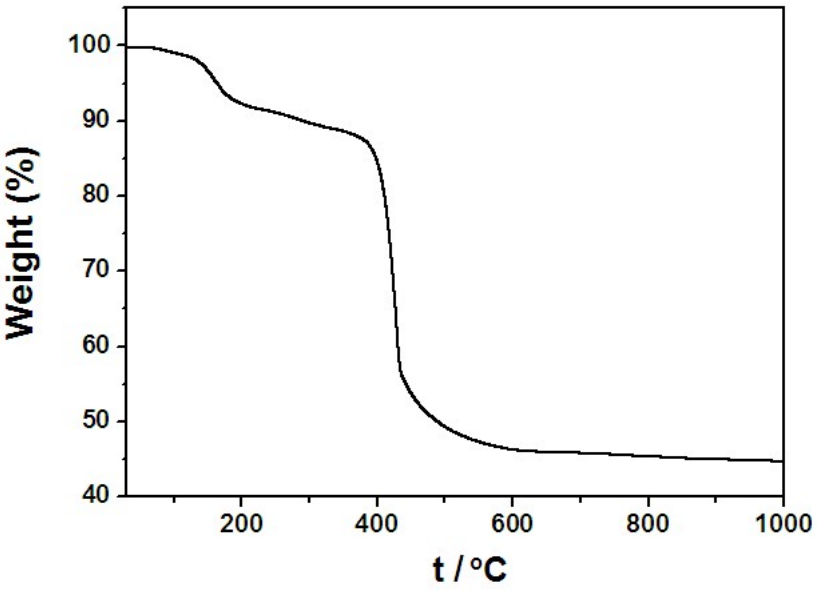

Fig. S6 The TG curve for complex **2**.

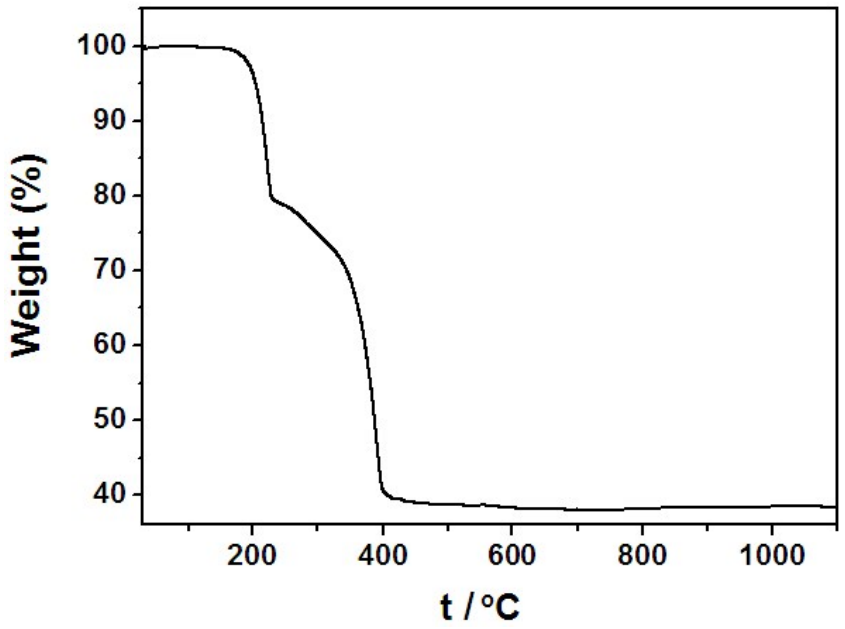

Fig. S7 The TG curve for complex **3**.

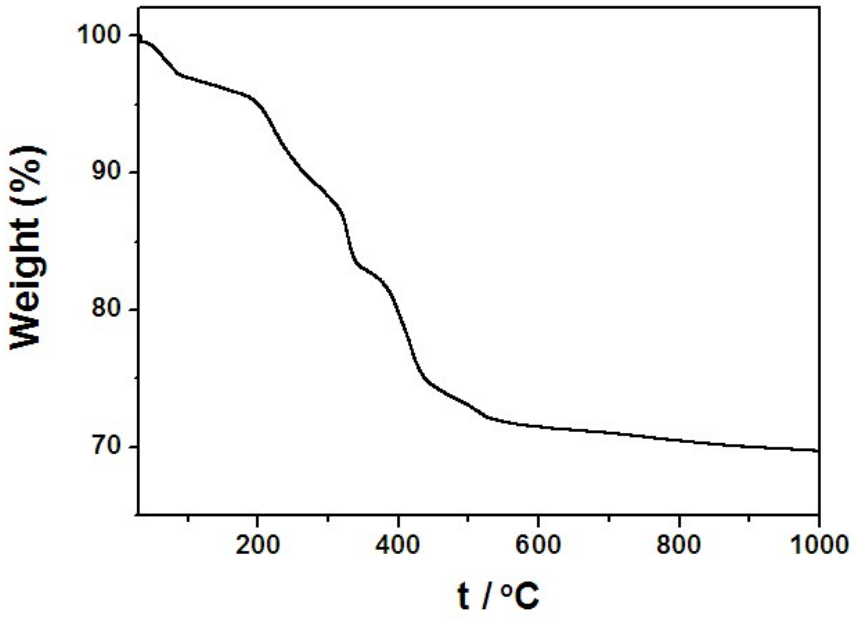

Fig. S8 The TG curve for complex **4**.

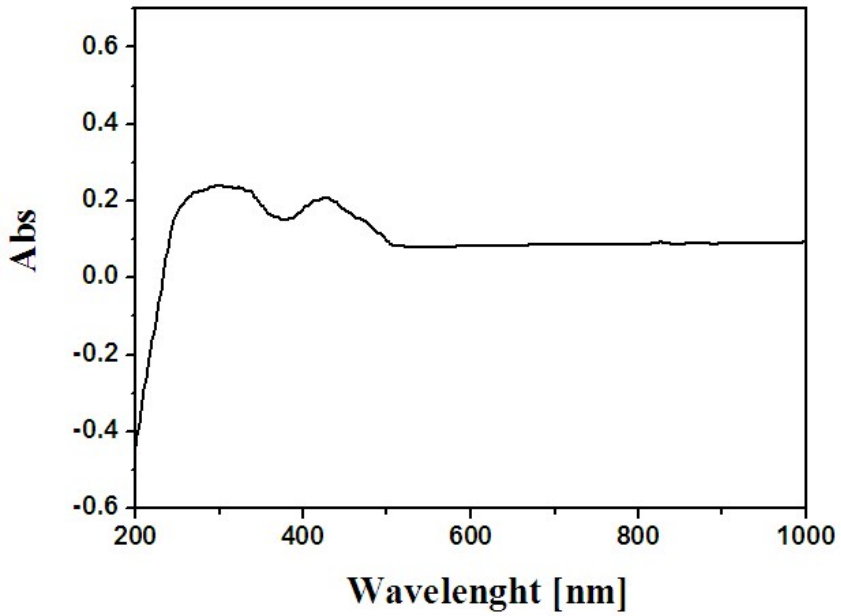

Fig. S9 The UV-Vis spectra for complex **1**.

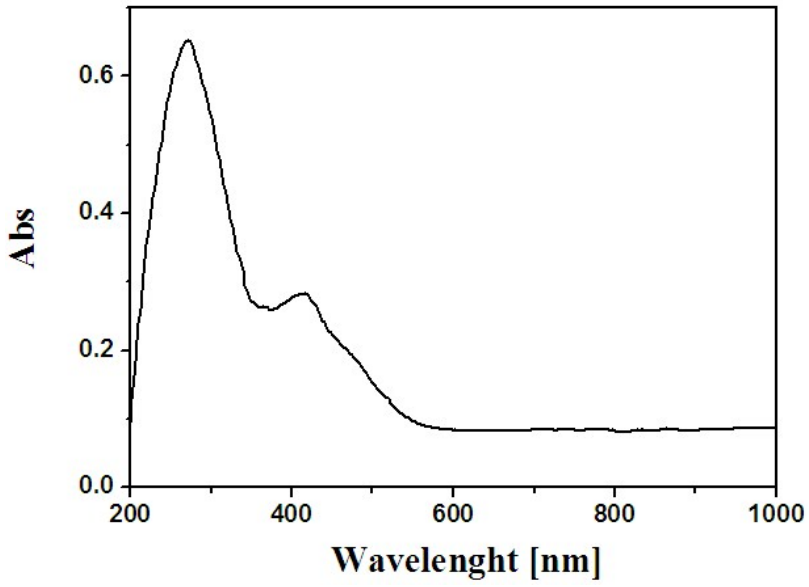

Fig. S10 The UV-Vis spectra for complex **2**.

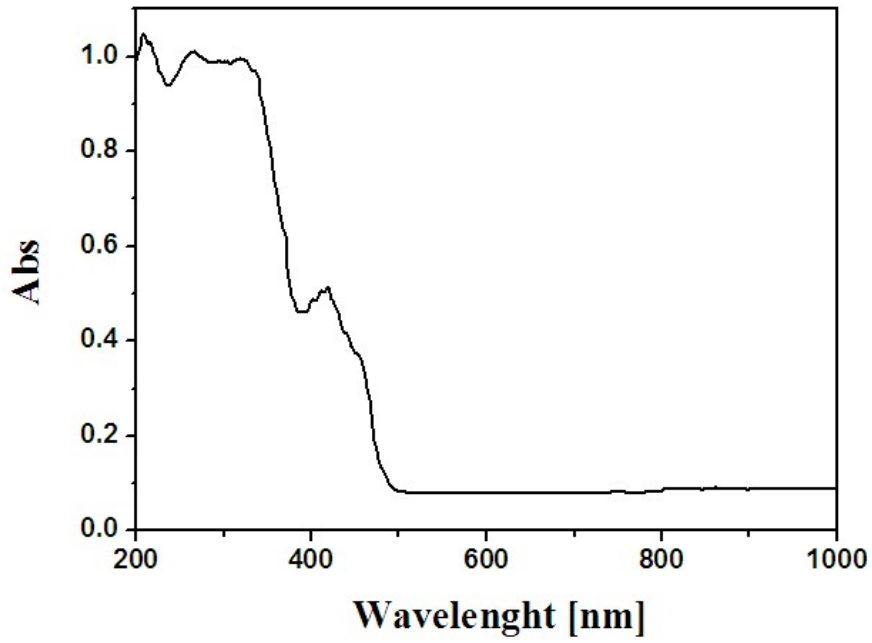

Fig. S11 The UV-Vis spectra for complex **3**.

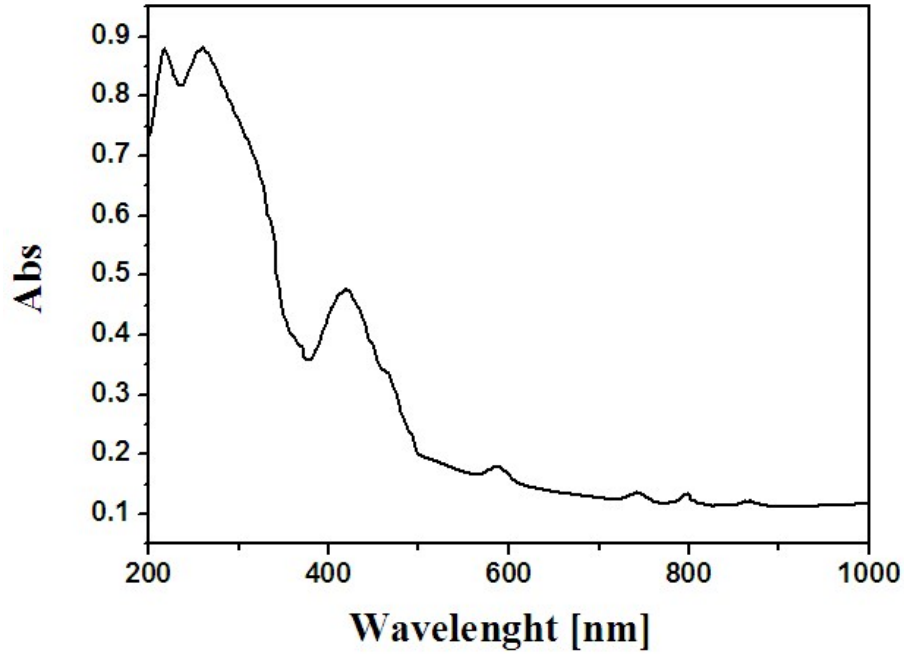

Fig. S12 The UV-Vis spectra for complex **4**.

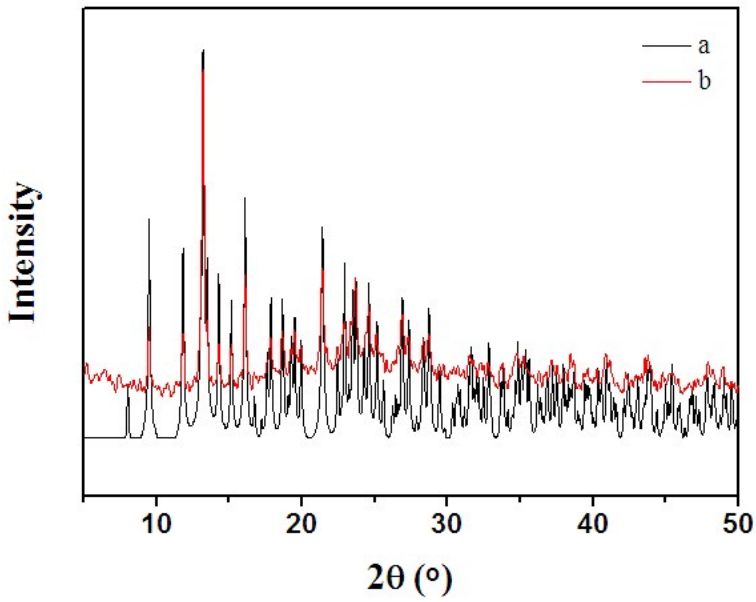

Fig. S13 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of complex **1**, (b) the experimental PXRD for complex **1**.

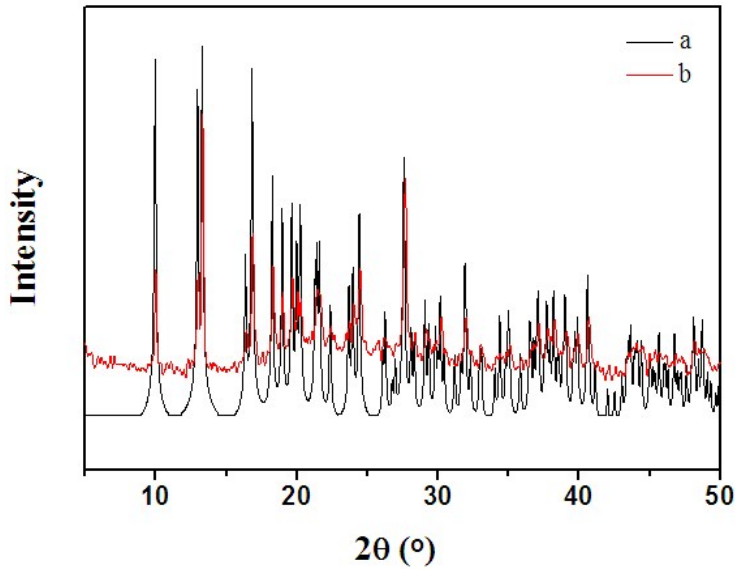

Fig. S14 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of complex **2**, (b) the experimental PXRD for complex **2**.

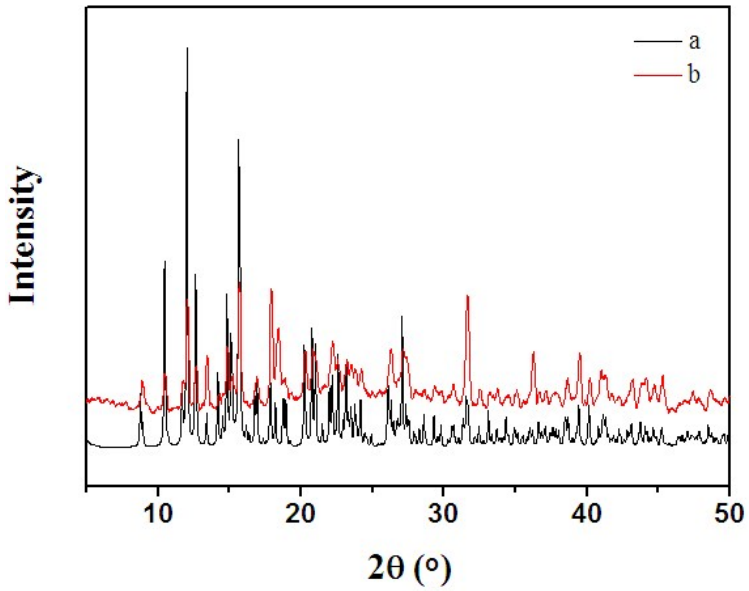

Fig. S15 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of complex **3**, (b) the experimental PXRD for complex **3**.

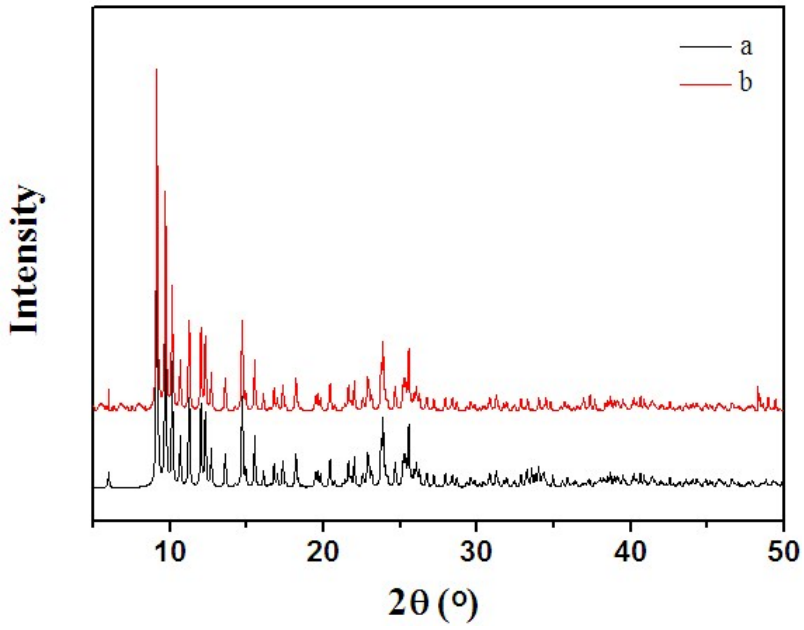

Fig. S16 PXRD powder patterns: (a) the simulated PXRD pattern calculated from single-crystal structure of complex **4**, (b) the experimental PXRD for complex **4**.