Supplementary materials

UO_2^{2+}-amino hybrid materials: Structural variation and photocatalysis properties

Xue-Ting Xu[1], Ya-Nan Hou[1], Si-Yue Wei[1], Xiao-Xi Zhang[1], Feng-Ying Bai[2], Li-Xian Sun[3], Zhan Shi[4], Yong-Heng Xing[1]*

[1] College of Chemistry and Chemical engineering, Liaoning Normal University, Huanghe Road 850#, Dalian City, 116029, P.R. China.

[2] College of Life Science, Liaoning Normal University, Dalian 11602, P.R. China

[3] Guangxi Key Laboratory of Information Materials, Guilin University of Electronic Technology, Guilin 541004, P.R. China

[4] State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, P.R. China

e-mail: xingyongheng2000@163.com tel: 0411-82156987

Table S1 the selected bond lengths (Å) and angles (°) of complex **1**

U2–O1	1.795(14)	U2–O2	1.786(14)	U1–O3	1.794(13)
U1–O4	1.771(14)	U2– O5	2.401(11)	U2$^{\#1}$-O6	2.258(10)
U2-O6	2.296(11)	U2-O10	2.492(13)	U2-O6$^{\#1}$	2.258(10)
U2-O9$^{\#1}$	2.373(15)	U2$^{\#1}$-O9	2.373(14)	U1-O5	2.323(11)
U1-O6	2.236(11)	U1-O8	2.373(15)	U1-O7$^{\#2}$	2.479(11)
U1-N1$^{\#2}$	2.596(15)	U1$^{\#2}$-N1	2.596(14)	U1$^{\#2}$-O7	2.479(11)
U1-O5-U2	106.2(4)	U1-O6-U2$^{\#1}$	138.3(5)	U1-O6-U2	112.9(4)
U2$^{\#1}$-O6-U2	108.4(5)	C1-O8-U1	139.7(13)	C3-O10-U2	144.8(13)
O4-U1-O3	174.0(6)	O4-U1-O6	92.6(6)	O3-U1-O6	93.3(5)
O4-U1-O5	93.6(6)	O3-U1-O5	89.2(6)	O6-U1-O5	71.4(4)
O4-U1-O8	90.6(7)	O3-U1-O8	88.6(7)	O6-U1-O8	88.1(5)
O5-U1-O8	159.3(5)	O4-U1-O7$^{\#2}$	89.2(6)	O3-U1-O7$^{\#2}$	86.6(5)
O6-U1-O7$^{\#2}$	143.3(4)	O5-U1-O7$^{\#2}$	71.9(4)	O8-U1-O7$^{\#2}$	128.5(5)
O4-U1-N1$^{\#2}$	82.5(6)	O3-U1-N1$^{\#2}$	91.7(6)	O6-U1-N1$^{\#2}$	154.4(4)
O5-U1-N1$^{\#2}$	133.8(4)	O8-U1-N1$^{\#2}$	66.9 (5)	O7$^{\#2}$-U1-N1$^{\#2}$	62.1(4)
O2-U2-O1	176.3(6)	O2-U2-O6$^{\#1}$	91.8(5)	O1-U2-O6$^{\#1}$	91.4(5)
O2-U2-O6	90.7(6)	O1-U2-O6	92.1(5)	O6$^{\#1}$-U2-O6	71.6(5)
O2-U2-O9$^{\#1}$	91.2(8)	O1-U2-O9$^{\#1}$	87.5(8)	O6$^{\#1}$-U2-O9$^{\#1}$	80.4(5)
O6-U2-O9$^{\#1}$	152.0(5)	O2-U2-O5	88.8(6)	O1-U2-O5	89.9(5)
O6$^{\#1}$-U2-O5	140.6(4)	O6-U2-O5	69.0(4)	O9$^{\#1}$-U2-O5	139.0(5)
O2-U2-O10	87.2(6)	O1-U2-O10	89.1(6)	O6$^{\#1}$-U2-O10	149.6(4)
O6-U2-O10	138.7(4)	O9$^{\#1}$-U2-O10	69.3(5)	O5-U2-O10	69.7(4)
O2-U2-U2$^{\#1}$	91.6(4)	O1-U2-U2$^{\#1}$	92.1(4)	O9$^{\#1}$-U2-U2$^{\#1}$	116.5(4)
O5-U2-U2$^{\#1}$	104.5(3)	O10-U2-U2$^{\#1}$	174.1(3)	C4-N1-U1$^{\#2}$	119.1(11)
C1-O9-U2$^{\#1}$	154.2(15)	C3-O7-U1$^{\#2}$	128.7(12)		

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

Table S2 the selected bond lengths (Å) and angles (°) of complex **2**

U2–O1	1.781(13)	U2–O2	1.778(12)	U1–O3	1.796(12)
U1–O4	1.788(12)	U2– O5	2.336(12)	U2–O5$^{\#1}$	2.373(12)
U1–O6	2.463(10)	U2–O6	2.474(11)	U1–O6$^{\#2}$	2.477(10)
U2–O7$^{\#3}$	2.247(10)	U1–O7	2.270(10)	U1–O7$^{\#4}$	2.292(11)
U2–O8	2.474(11)	U1–O9	2.368(12)	U2–O7$^{\#5}$	2.247(10)
U2-O5-U2$^{\#1}$	115.3(5)	U1-O6-U2	132.2(4)	U1-O6-U1$^{\#2}$	110.2(4)
U2-O6-U1$^{\#2}$	98.8(4)	U2$^{\#3}$-O7-U1	141.1(5)	U2$^{\#3}$-O7-U1$^{\#4}$	111.8(4)
U1-O7-U1$^{\#4}$	107.1(4)	C1-O8-U2	139.8(11)	C1-O9-U1	143.3(12)
O4-U1-O3	176.5(5)	O4-U1-O7	89.9(4)	O3-U1-O7	92.7(4)
O4-U1-O7$^{\#4}$	92.9(5)	O3-U1-O7$^{\#4}$	90.1(4)	O7-U1-O7$^{\#4}$	70.3(4)
O4-U1-O9	93.7(5)	O3-U1-O9	84.5(4)	O7-U1-O9	79.5(4)
O7$^{\#4}$-U1-O9	149.0(4)	O4-U1-O6	83.8(4)	O3-U1-O6	92.9(4)
O7-U1-O6	150.6(4)	O7$^{\#4}$-U1-O6	138.5(3)	O9-U1-O6	72.3(4)

O4-U1-O6$^{\#2}$	94.8(4)	O3-U1-O6$^{\#2}$	84.7(4)	O7-U1-O6$^{\#2}$	140.6(4)
O7$^{\#4}$-U1-O6$^{\#2}$	70.5(3)	O9-U1-O6$^{\#2}$	138.8(4)	O6-U1-O6$^{\#2}$	68.7(4)
O2-U2-O1	175.8(6)	O2-U2-O7$^{\#5}$	91.7(5)	O1-U2-O7$^{\#5}$	90.4(5)
O2-U2-O5	88.3(5)	O1-U2-O5	95.7(6)	O7$^{\#5}$-U2-O5	80.6(4)
O2-U2-O5$^{\#1}$	89.5(5)	O1-U2-O5$^{\#1}$	90.8(5)	O7$^{\#5}$-U2-O5$^{\#1}$	145.2(4)
O5-U2-O5$^{\#1}$	64.7(5)	O2-U2-O6	84.0(5)	O1-U2-O6	93.2(5)
O7$^{\#5}$-U2-O6	51.7(3)	O5-U2-O6	150.5(4)	O5$^{\#1}$-U2-O6	143.3(4)
O2-U2-O8	95.3(5)	O1-U2-O8	80.9(5)	O7$^{\#5}$-U2-O8	145.4(4)
O5-U2-O8	133.3(4)	O5$^{\#1}$-U2-O8	68.8(4)	O6-U2-O8	75.9(4)

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

Table S3 the selected bond lengths (Å) and angles (°) of complex **3**

U1–O2	1.763(5)	U1–O1	1.769(5)	U1–O3	2.273(6)
U1–O3$^{\#1}$	2.291(6)	U1– O4	2.468(4)	U1–O5	2.484(4)
U1–N1	2.612(4)	U1–N2	2.654(5)	C1–N1	1.336(8)
C5–N1	1.348(7)	C6–N2	1.355(7)	C10–N2	1.350(7)
C11–O5	1.244(7)	C11–O4	1.253(7)	O3–U1$^{\#1}$	2.291(6)
O2-U1-O1	174.7(3)	O2-U1-O3	90.5(4)	O1-U1-O3	94.9(4)
O2-U1-O3$^{\#1}$	91.2(4)	O1-U1-O3$^{\#1}$	93.2(4)	O2-U1-O4	90.48(19)
O1-U1-O4	86.7(2)	O3-U1-O4	120.6(16)	O3$^{\#1}$-U1-O4	157.13(17)
O2-U1-O5	90.2(2)	O1-U1-O5	91.6(2)	O3-U1-O5	69.04(17)
O3$^{\#1}$-U1-O5	105.6(18)	O4-U1-O5	51.58(15)	O2-U1-N1	96.15(17)
O1-U1-N1	82.37(18)	O3-U1-N1	107.61(17)	O3$^{\#1}$-U1-N1	71.19(18)
O4-U1-N1	131.24(14)	O5-U1-N1	172.92(17)	O2-U1-N2	80.7(2)
O1-U1-N2	94.1(2)	O3-U1-N2	165.0(2)	O3$^{\#1}$-U1-N2	130.79(17)
O4-U1-N2	71.94(13)	O5-U1-N2	122.73(14)	N1-U1-N2	61.75(14)
O3$^{\#1}$-O3-U1	72.4(5)	O3$^{\#1}$-O3-U1$^{\#1}$	71.0(5)	U1-O3-U1$^{\#1}$	143.4(3)
C11-O4-U1	94.8(3)	C11-O5-U1	94.3(4)	C1-N1-C5	117.8(5)
C1-N1-U1	119.3(4)	C5-N1-U1	122.6(4)	C10-N2-C6	117.9(5)
C10-N2-U1	120.5(4)	C6-N2-U1	120.5(4)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1

Table S4 the selected bond lengths (Å) and angles (°) of complex **4**

U1-O2	1.755(3)	U1-O1	1.760(3)	U1-O3	2.437(3)
U1-O5	2.445(3)	U1-O6	2.457(3)	U1-O4	2.472(3)
U1-N1	2.632(4)	U1-N2	2.643(4)		
O2-U1-O1	179.08(15)	O2-U1-O3	89.03(14)	O1-U1-O3	90.26(14)
O2-U1-O5	92.23(13)	O1-U1-O5	88.03(13)	O3-U1-O5	67.09(12)
O2-U1-O6	83.88(14)	O1-U1-O6	96.97(14)	O3-U1-O6	118.69(11)
O5-U1-O6	52.55(11)	O2-U1-O4	94.30(14)	O1-U1-O4	84.81(14)
O3-U1-O4	52.62(10)	O5-U1-O4	119.12(11)	O6-U1-O4	171.24(10)

O2-U1-N1	103.57(13)	O1-U1-N1	77.10(13)	O3-U1-N1	166.82(12)
O5-U1-N1	115.46(12)	O6-U1-N1	67.36(11)	O4-U1-N1	121.35(11)
O2-U1-N2	77.47(12)	O1-U1-N2	102.39(12)	O3-U1-N2	119.69(12)
O5-U1-N2	167.14(12)	O6-U1-N2	117.77(11)	O4-U1-N2	69.95(11)

Table S5 Bond Distances (Å) and Angles (°) of Hydrogen Bonds in Complexes **1-4***

D-H···A	d (D-H) Å	d (H···A) Å	d (D···A) Å	∠DHA(°)
		Complex **1**		
N1-H1A···O3$^{\#1}$	0.90	2.20	3.031(2)	153
N2-H2D···O1$^{\#2}$	0.86	2.00	2.820(3)	158
C7-H7···O2$^{\#3}$	0.93	2.28	2.998(16)	134
		Complex **2**		
N1-H1B···O3$^{\#4}$	0.86	2.29	2.979(18)	137
O2W-H2WA···O4$^{\#5}$	0.90	2.03	2.918(16)	169
O2W-H2WB···O4$^{\#6}$	0.90	2.09	2.918(16)	152
C2-H2B···O1$^{\#7}$	0.97	2.45	3.226(11)	137
C2-H2B···O9$^{\#8}$	0.97	2.39	3.192(11)	140
O1W-H1WA···N1	0.90	2.09	2.819(19)	137
		Complex **3**		
C1-H1···O5$^{\#9}$	0.93	2.57	3.283(2)	134
C2-H2···O1$^{\#10}$	0.93	2.47	3.399(2)	176
		Complex **4**		
C14-H14C···O2$^{\#11}$	0.96	2.42	3.378(18)	174

*Symmetry transformation used to generate equivalent atoms: #1: x+1/2, y+1/2, z; #2: 3/2-x, 3/2-y, 1-z; #3: 3/2-x, 1/2+y, 1/2-z; #4: 1/2-x, 3/2-y, 1-z; #5: x+1, y-1, z; #6: 1-x, y-1, 1/2-z; #7: 3/2-x, 1/2-y, -z; #8: 5/2-x, 1/2-y, -z; #9: -x, 1-y, -z: #10: x-1/2, 1/2-y, -z; #11: x+1/2, 1/2-y, 1/2+z.

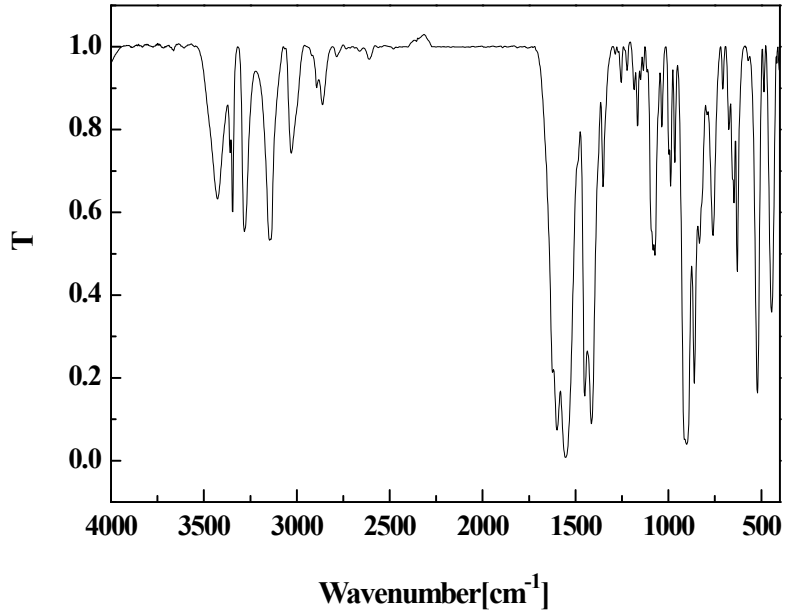

Fig. S1 The IR spectra of complex **1**

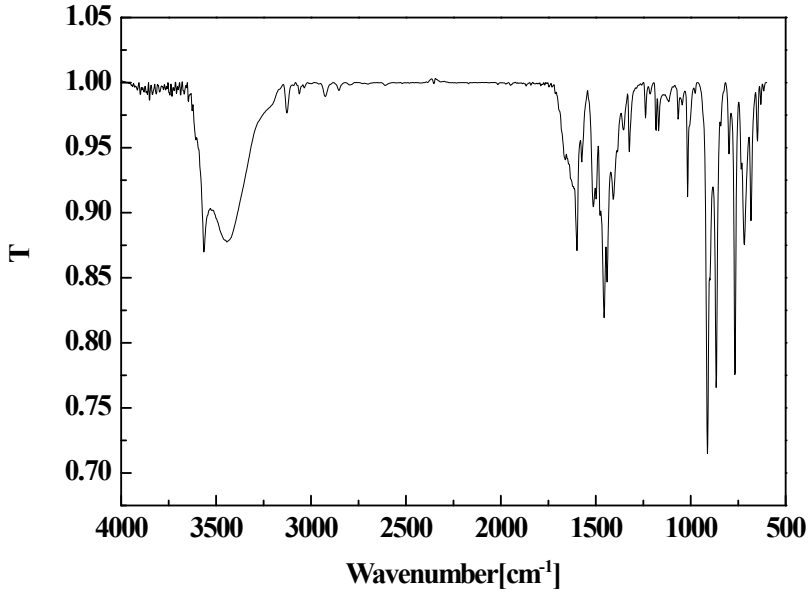

Fig. S2 The IR spectra of complex **2**

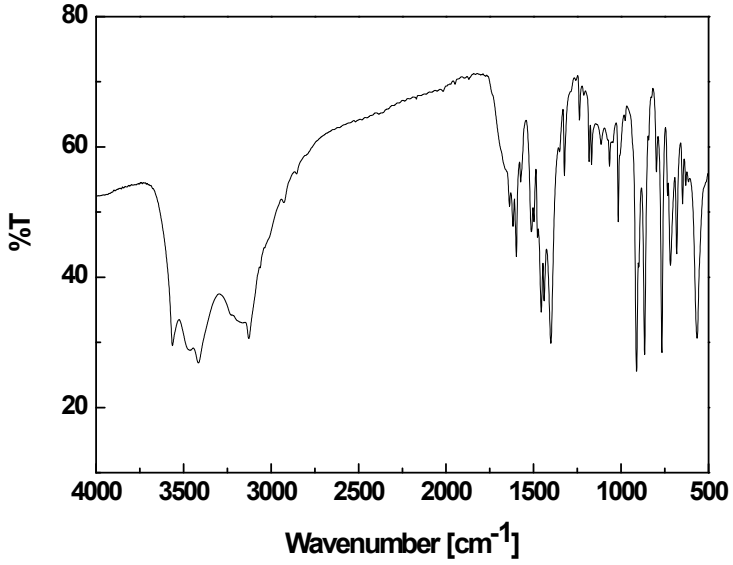

Fig. S3 The IR spectra of complex **3**

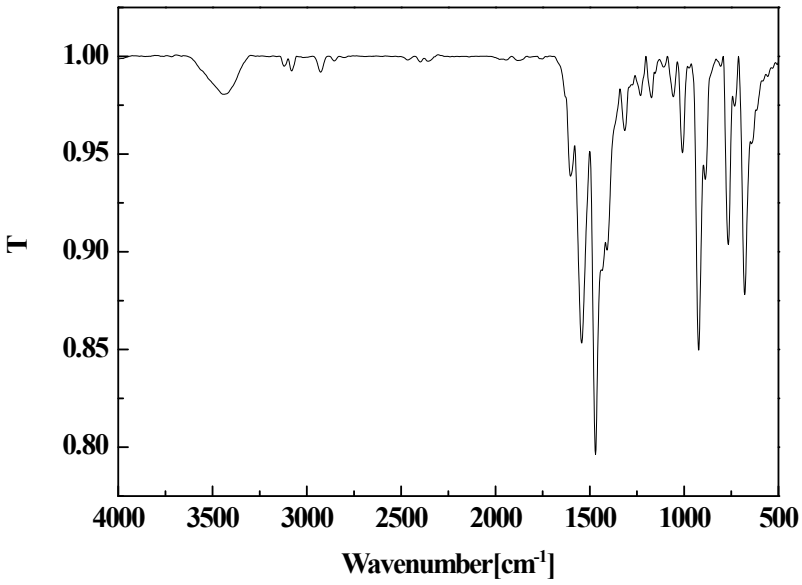

Fig. S4 The IR spectra of complex **4**

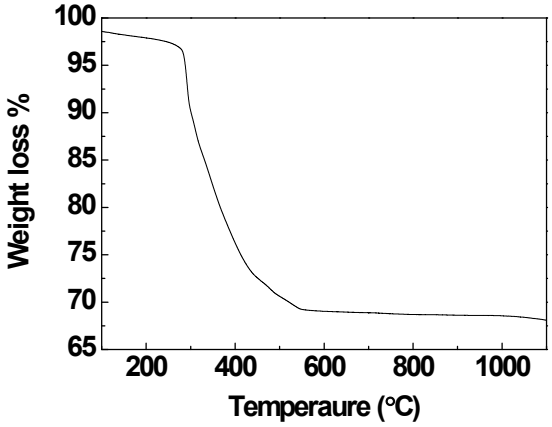

Fig. S5 The TG curve of the uranyl complex **1**

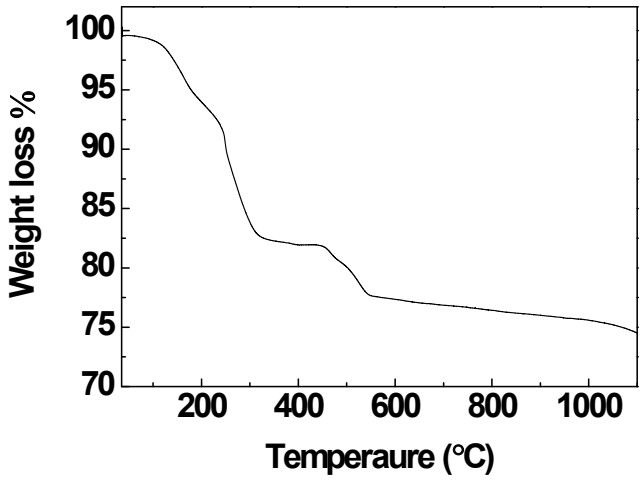

Fig. S6 The TG curve of the uranyl complex **2**

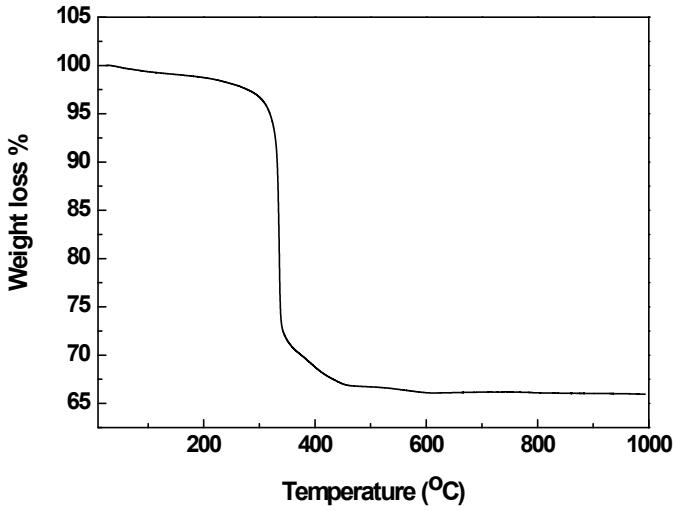

Fig. S7 The TG curve of the uranyl complex **3**

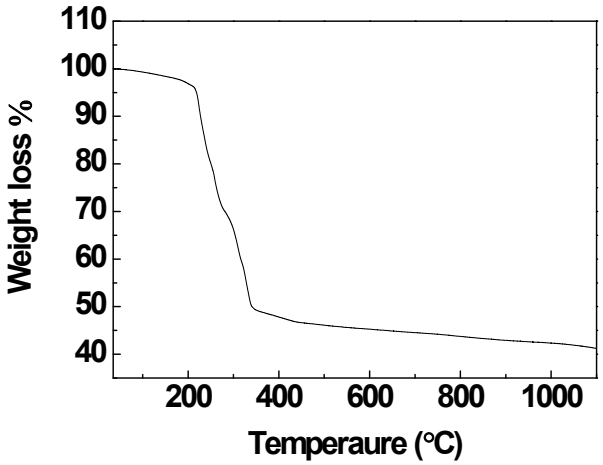

Fig. S8 The TG curve of the uranyl complex **4**

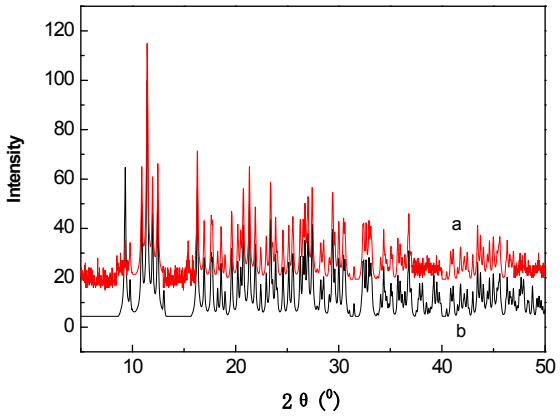

Fig. S9 The experimental PXRD(a) and simulation PXRD(b) of complex **1**

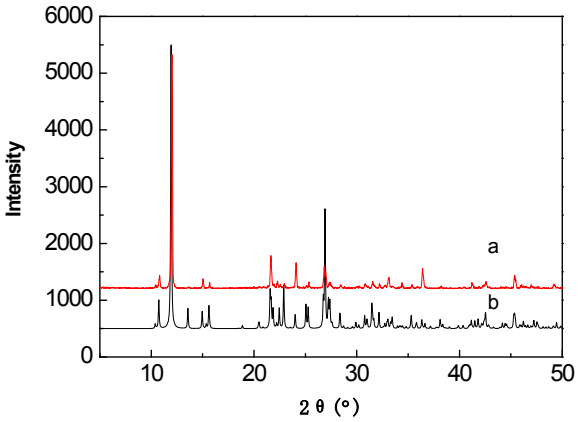

Fig. S10 The experimental PXRD(a) and simulation PXRD(b) of complex **2**

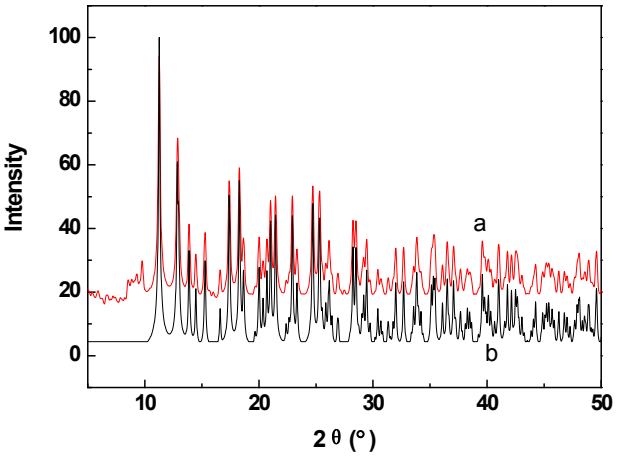

Fig. S11 The experimental PXRD(a) and simulation PXRD(b) of complex **3**

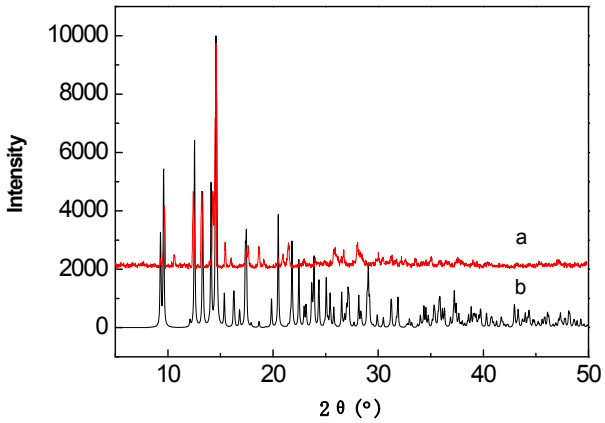

Fig. S12 The experimental PXRD(a) and simulation PXRD(b) of complex **4**

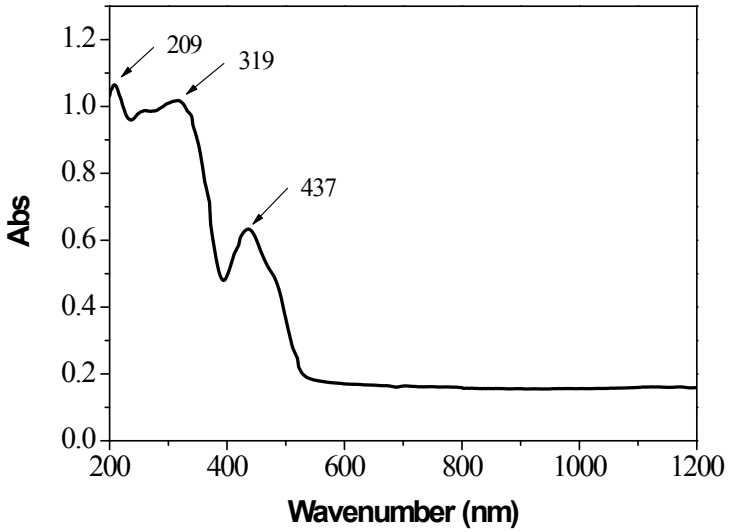

Fig S13 The solid UV-Vis spectra of the uranyl complex **1**

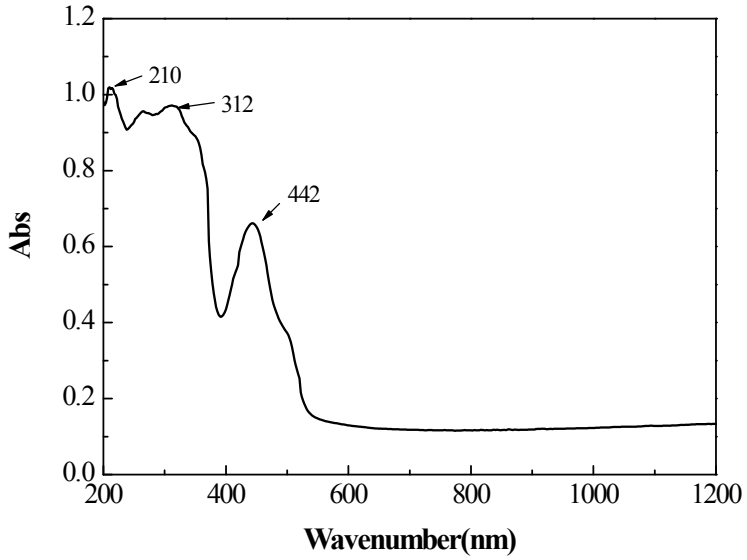

Fig. S14 The solid UV-Vis spectra of the uranyl complex **2**

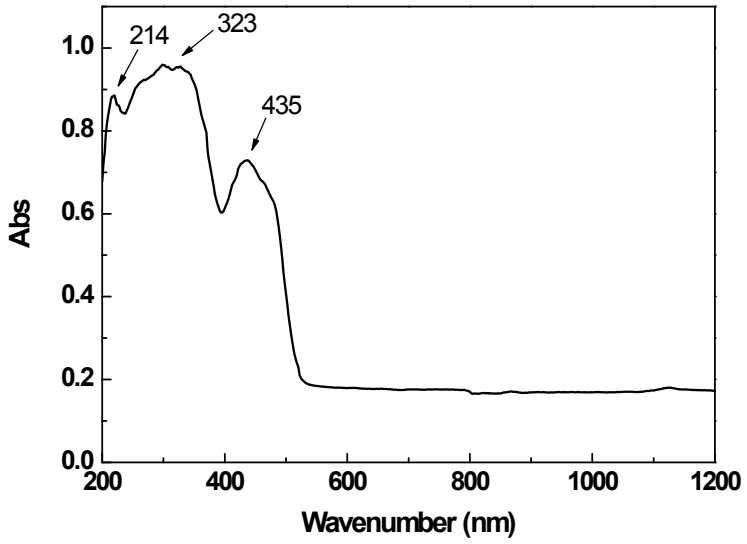

Fig. S15 The solid UV-Vis spectra of the uranyl complex **3**

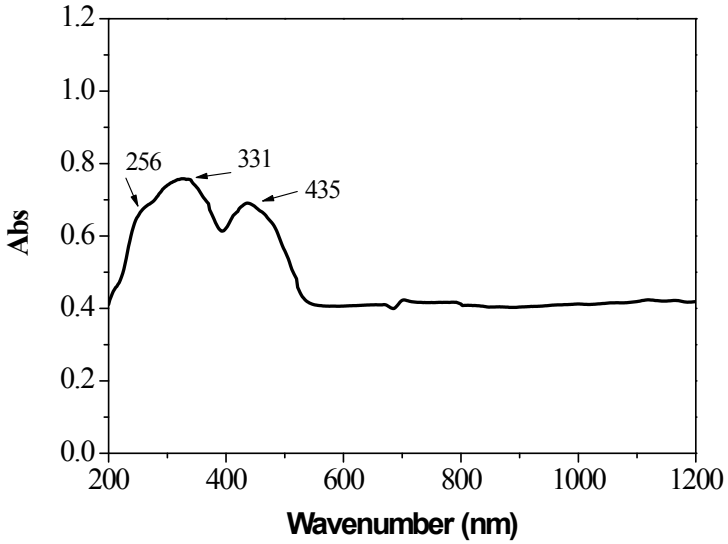

Fig. S16 The solid UV-Vis spectra of the uranyl complex **4**

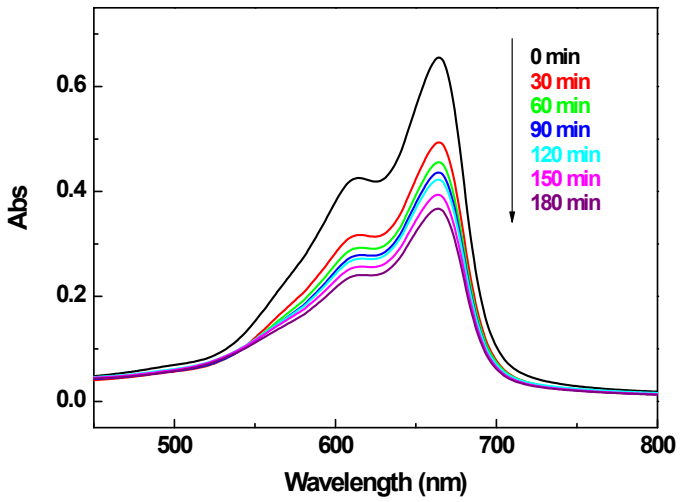

Fig. S17 Absorption spectra of methylene blue solution during the photodegradation reaction under the irradiation of visible light with the use of complex **2**

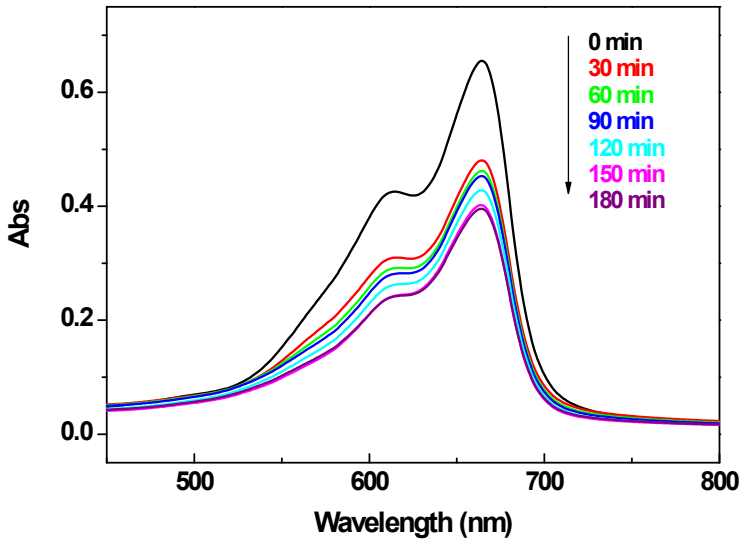

Fig. S18 Absorption spectra of methylene blue solution during the photodegradation reaction under the irradiation of UV light with the use of complex **2**

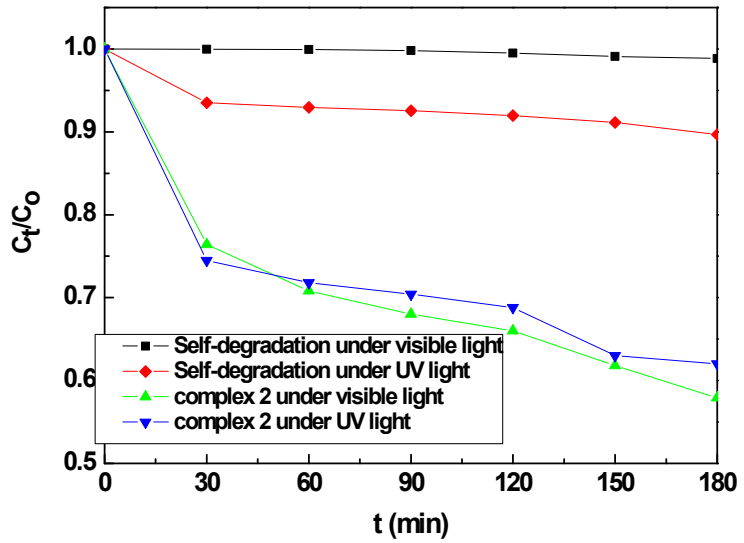

Fig. S19 Self-degradation and photocatalytic decomposition of methylene blue solution with the use of complex **2** under UV and visible light

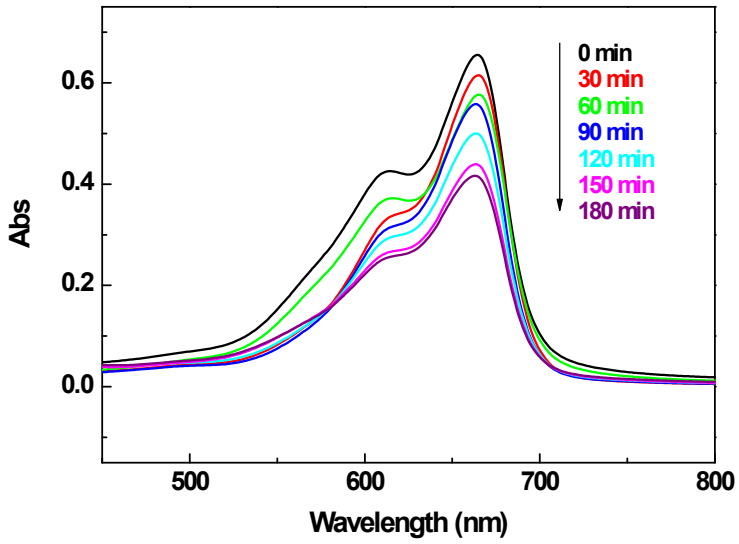

Fig. S20 Absorption spectra of methylene blue solution during the photodegradation reaction under the irradiation of visible light with the use of complex **3**

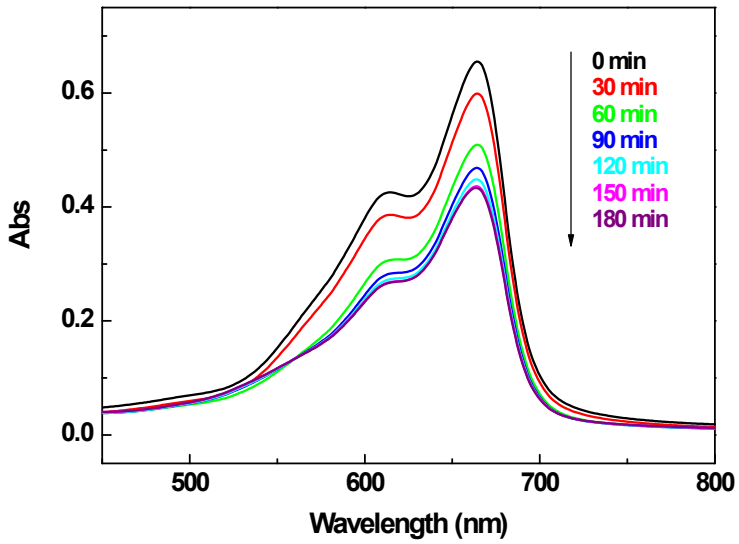

Fig. S21 Absorption spectra of methylene blue solution during the photodegradation reaction under the irradiation of UV light with the use of complex **3**

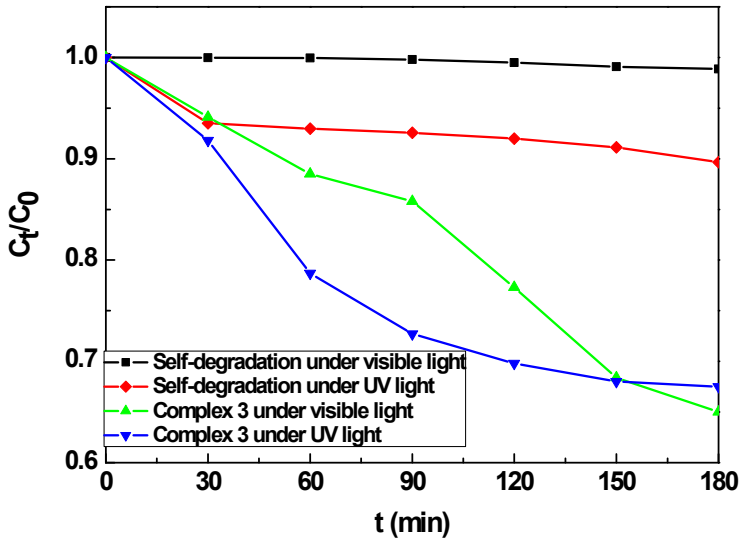

Fig. S22 Self-degradation and photocatalytic decomposition of methylene blue solution with the use of complex **3** under UV and visible light

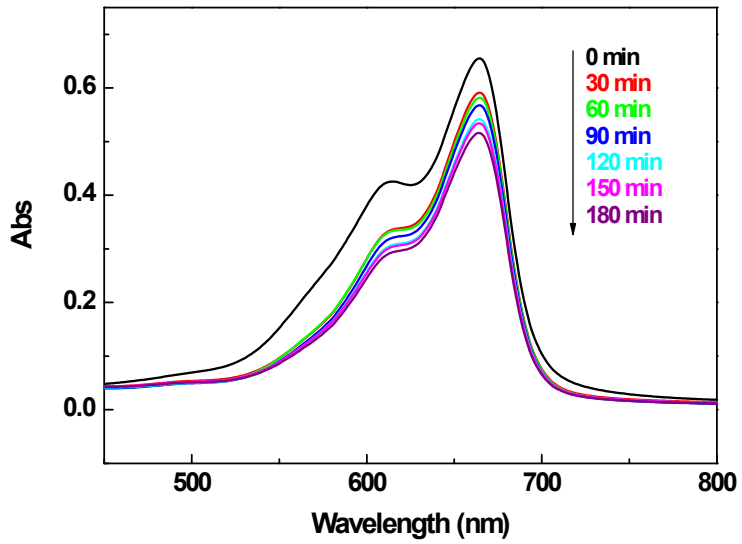

Fig. S23 Absorption spectra of methylene blue solution during the photodegradation reaction under the irradiation of visible light with the use of complex **4**

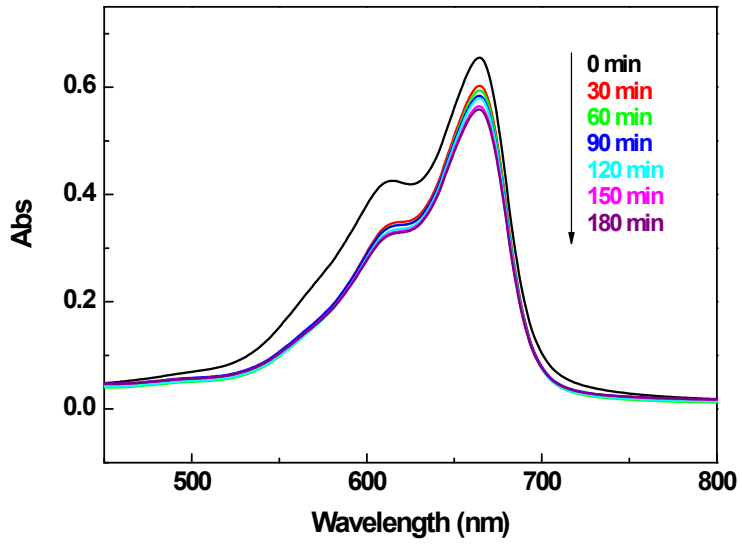

Fig. S24 Absorption spectra of methylene blue solution during the photodegradation reaction under the irradiation of UV light with the use of complex **4**

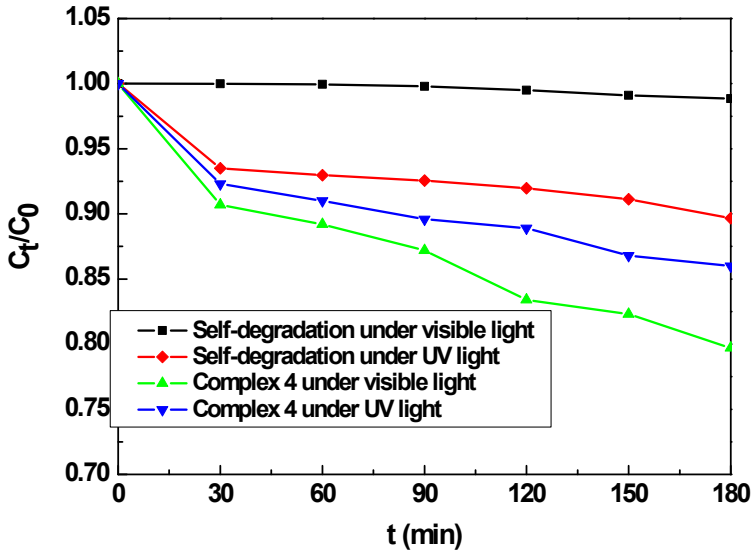

Fig. S25 Self-degradation and photocatalytic decomposition of methylene blue solution with the use of complex **4** under UV and visible light