Supporting information

A Uranium-Zinc-Organic Molecular Compound Containing Planar Tetranuclear Uranyl Units

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Table S1. Crystal data and structure refinement for $Zn_2(phen)_4U_4O_{10}(OAc)_2(NA)_2(QA)_2$.

Empirical formula	$C_{39}H_{26}N_6O_{13}U_2Zn$	
Formula weight	1328.09	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/C$	
Unit cell dimensions	a = 12.9751(6) Å	α = 90°
	b = 20.3412(8) Å	β = 92.2870(10)°
	c = 14.6543(6) Å	γ = 90°
Volume	3864.6(3) $Å^3$	
Z	4	
Calculated density	2.283 Mg/m^3	
Absorption coefficient	9.053 mm^{-1}	
F(000)	2480	
Crystal size	0.45 × 0.45 × 0.20 mm	
Theta range for data collection	1.71 to 23.29°	
Limiting indices	-11≤h≤14, -22≤k≤22, -16≤l≤16	
Reflections collected / unique	18371 / 5563 [R(int) = 0.0444]	
Completeness to theta = 23.29	99.7 %	
Max. and min. transmission	0.4062 and 0.1819	
Refinement method	Full-matrix least-squares on F^2	
Data / parameters	5563 / 550	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0247, wR2 = 0.0577	
Largest diff. peak and hole	1.104 and -0.883 e. $Å^{-3}$	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Zn_2(phen)_4U_4O_{10}(OAc)_2(NA)_2(QA)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)[a]
U(1)	4224(1)	4378(1)	-4439(1)	25(1)
U(2)	7202(1)	4103(1)	-4296(1)	32(1)
Zn(1)	2506(1)	3622(1)	-985(1)	31(1)
O(1)	3386(3)	3486(2)	-3660(2)	32(1)
O(2)	2446(3)	3614(2)	-2438(3)	34(1)
O(3)	5557(3)	3606(2)	-3768(3)	38(1)
O(4)	5489(4)	2514(2)	-3965(3)	44(1)
O(5)	7553(4)	3086(2)	-3367(3)	58(1)
O(6)	8897(3)	3595(2)	-3855(3)	54(1)
O(7)	2463(4)	4733(3)	-4536(4)	79(2)
O(8)	1316(4)	5436(3)	-4922(4)	70(2)
O(9)	5843(3)	4669(2)	-4767(3)	32(1)
O(10)	4345(3)	4806(2)	-3380(2)	40(1)
O(11)	4027(3)	3896(2)	-5440(3)	36(1)
O(12)	7369(4)	4600(2)	-3314(3)	56(1)
O(13)	7108(3)	3601(2)	-5274(3)	46(1)
N(1)	3867(4)	3079(2)	-1340(3)	30(1)
N(2)	10870(6)	2106(4)	-2925(5)	81(2)
N(3)	928(4)	4013(2)	-992(3)	39(1)
N(4)	1610(4)	2770(2)	-730(3)	37(1)
N(5)	3035(4)	3795(2)	434(3)	37(1)
N(6)	3093(4)	4614(2)	-1013(3)	31(1)
C(1)	4105(4)	3153(2)	-2224(3)	24(1)
C(2)	5024(4)	2927(2)	-2549(3)	27(1)
C(3)	5688(5)	2574(3)	-1956(4)	35(1)
C(4)	5428(5)	2479(3)	-1067(4)	38(2)
C(5)	4518(5)	2748(3)	-783(4)	38(2)
C(6)	3250(4)	3448(2)	-2815(4)	27(1)
C(7)	5360(4)	3002(3)	-3520(4)	30(1)
C(8)	10233(6)	2616(3)	-3142(5)	52(2)
C(9)	9175(5)	2539(3)	-3235(4)	44(2)
C(10)	8782(7)	1927(4)	-3100(6)	71(2)
C(11)	9400(9)	1399(4)	-2901(7)	88(3)
C(12)	10418(9)	1515(5)	-2813(7)	90(3)
C(13)	8500(5)	3102(3)	-3490(4)	42(2)
C(14)	916(6)	4696(4)	-3755(5)	59(2)
C(15)	1608(5)	4968(3)	-4432(4)	35(1)

C(16)	598(6)	4618(3)	-1134(5)	57(2)
C(17)	-453(7)	4781(4)	-1238(7)	79(3)
C(18)	-1150(6)	4305(4)	-1186(6)	69(2)
C(19)	-857(5)	3655(3)	-1023(5)	50(2)
C(20)	202(5)	3532(3)	-930(4)	36(1)
C(21)	576(5)	2868(3)	-776(4)	37(1)
C(22)	-139(5)	2358(3)	-699(4)	47(2)
C(23)	260(7)	1728(4)	-551(5)	62(2)
C(24)	1300(7)	1630(3)	-491(5)	64(2)
C(25)	1952(5)	2167(3)	-598(4)	48(2)
C(26)	-1556(5)	3118(4)	-940(5)	64(2)
C(27)	-1214(6)	2507(4)	-780(5)	63(2)
C(28)	3029(6)	3391(3)	1131(4)	52(2)
C(29)	3373(6)	3574(4)	2019(4)	57(2)
C(30)	3722(6)	4200(4)	2183(4)	53(2)
C(31)	3743(5)	4640(3)	1453(4)	39(2)
C(32)	3393(4)	4416(3)	584(4)	32(1)
C(33)	3422(4)	4852(3)	-190(4)	32(1)
C(34)	3773(5)	5501(3)	-67(5)	41(2)
C(35)	3790(6)	5910(3)	-852(5)	49(2)
C(36)	3472(6)	5666(3)	-1667(5)	48(2)
C(37)	3115(5)	5014(3)	-1737(4)	37(2)
C(38)	4104(5)	5302(4)	1553(5)	51(2)
C(39)	4116(5)	5715(3)	828(5)	49(2)

Table S3. Bond lengths [Å] and angles [º] for $Zn_2(phen)_4U_4O_{10}(OAc)_2(NA)_2(QA)_2$[a].

U(1)-O(11)	1.775(4)	U(2)-O(13)	1.760(4)
U(1)-O(10)	1.780(4)	U(2)-O(12)	1.765(4)
U(1)-O(9)	2.253(4)	U(2)-O(9)	2.193(4)
U(1)-O(9)#1	2.262(3)	U(2)-O(8)#1	2.462(5)
U(1)-O(7)	2.395(5)	U(2)-O(6)	2.492(4)
U(1)-O(1)	2.425(4)	U(2)-O(5)	2.509(4)
U(1)-O(3)	2.507(4)	U(2)-O(3)	2.511(4)
Zn(1)-O(2)	2.128(4)	Zn(1)-N(1)	2.164(5)
Zn(1)-N(4)	2.128(5)	Zn(1)-N(5)	2.192(5)
Zn(1)-N(6)	2.158(5)	Zn(1)-N(3)	2.196(5)
O(11)-U(1)-O(10)	174.45(18)	O(13)-U(2)-O(12)	176.9(2)
O(11)-U(1)-O(9)	94.21(16)	O(13)-U(2)-O(9)	91.09(18)
O(10)-U(1)-O(9)	90.42(17)	O(12)-U(2)-O(9)	91.59(18)
O(11)-U(1)-O(9)#1	92.65(15)	O(13)-U(2)-O(8)#1	82.7(2)
O(10)-U(1)-O(9)#1	91.71(16)	O(12)-U(2)-O(8)#1	95.1(2)

O(9)-U(1)-O(9)#1	71.49(15)	O(9)-U(2)-O(8)#1	106.68(15)
O(11)-U(1)-O(7)	90.6(2)	O(13)-U(2)-O(6)	90.13(18)
O(10)-U(1)-O(7)	87.4(2)	O(12)-U(2)-O(6)	87.00(19)
O(9)-U(1)-O(7)	143.50(16)	O(9)-U(2)-O(6)	171.58(14)
O(9)#1-U(1)-O(7)	72.17(16)	O(8)#1-U(2)-O(6)	65.23(15)
O(11)-U(1)-O(1)	85.59(15)	O(13)-U(2)-O(5)	88.18(18)
O(10)-U(1)-O(1)	88.93(15)	O(12)-U(2)-O(5)	90.9(2)
O(9)-U(1)-O(1)	137.45(13)	O(9)-U(2)-O(5)	136.85(14)
O(9)#1-U(1)-O(1)	151.05(13)	O(8)#1-U(2)-O(5)	115.98(16)
O(7)-U(1)-O(1)	78.96(17)	O(6)-U(2)-O(5)	51.53(14)
O(11)-U(1)-O(3)	93.04(16)	O(13)-U(2)-O(3)	89.13(17)
O(10)-U(1)-O(3)	85.94(17)	O(12)-U(2)-O(3)	93.29(19)
O(9)-U(1)-O(3)	67.26(12)	O(9)-U(2)-O(3)	68.02(12)
O(9)#1-U(1)-O(3)	138.65(13)	O(8)#1-U(2)-O(3)	170.23(16)
O(7)-U(1)-O(3)	148.60(17)	O(6)-U(2)-O(3)	120.33(13)
O(1)-U(1)-O(3)	70.27(13)	O(5)-U(2)-O(3)	68.82(13)
O(2)-Zn(1)-N(4)	99.85(17)	N(6)-Zn(1)-N(5)	76.71(18)
O(2)-Zn(1)-N(6)	89.27(16)	N(1)-Zn(1)-N(5)	94.73(18)
N(4)-Zn(1)-N(6)	163.88(18)	O(2)-Zn(1)-N(3)	90.10(17)
O(2)-Zn(1)-N(1)	75.68(15)	N(4)-Zn(1)-N(3)	77.31(19)
N(4)-Zn(1)-N(1)	94.77(18)	N(6)-Zn(1)-N(3)	89.50(18)
N(6)-Zn(1)-N(1)	100.39(17)	N(1)-Zn(1)-N(3)	162.45(18)
O(2)-Zn(1)-N(5)	161.45(17)	N(5)-Zn(1)-N(3)	101.69(19)
N(4)-Zn(1)-N(5)	96.71(18)		

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

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Zn_2(phen)_4U_4O_{10}(OAc)_2(NA)_2(QA)_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U11+ ... + 2hkabU12]$.

	U11	U22	U33	U23	U13	U12
U(1)	25(1)	25(1)	25(1)	3(1)	1(1)	3(1)
U(2)	25(1)	34(1)	36(1)	1(1)	-1(1)	7(1)
Zn(1)	30(1)	29(1)	35(1)	0(1)	3(1)	-3(1)
O(1)	29(2)	38(2)	28(2)	7(2)	0(2)	0(2)
O(2)	29(2)	41(2)	33(2)	3(2)	2(2)	3(2)
O(3)	28(2)	39(2)	46(2)	20(2)	4(2)	6(2)
O(4)	61(3)	42(3)	31(2)	-7(2)	4(2)	5(2)
O(5)	31(3)	66(3)	76(3)	30(3)	3(2)	10(2)
O(6)	31(3)	53(3)	77(3)	27(3)	1(2)	7(2)
O(7)	28(3)	69(4)	140(5)	-4(3)	8(3)	11(3)
O(8)	64(4)	68(3)	79(4)	40(3)	0(3)	-5(3)
O(9)	25(2)	30(2)	42(2)	12(2)	6(2)	4(2)
O(10)	44(3)	45(2)	31(2)	-7(2)	7(2)	-1(2)
O(11)	42(3)	34(2)	33(2)	-1(2)	2(2)	0(2)

O(12)	52(3)	62(3)	52(3)	-16(2)	-9(2)	13(2)
O(13)	41(3)	44(3)	53(3)	-8(2)	4(2)	7(2)
N(1)	31(3)	31(3)	27(2)	0(2)	3(2)	-4(2)
N(2)	66(5)	89(6)	87(5)	-5(4)	-9(4)	35(4)
N(3)	30(3)	38(3)	49(3)	3(2)	9(2)	0(2)
N(4)	38(3)	34(3)	40(3)	8(2)	1(2)	-6(2)
N(5)	42(3)	35(3)	35(3)	0(2)	5(2)	-2(2)
N(6)	24(3)	32(3)	36(3)	-1(2)	5(2)	-4(2)
C(1)	29(3)	19(3)	25(3)	0(2)	0(2)	-2(2)
C(2)	34(3)	20(3)	27(3)	3(2)	-5(3)	-4(2)
C(3)	38(4)	34(3)	31(3)	4(3)	-4(3)	9(3)
C(4)	42(4)	42(4)	32(3)	9(3)	-1(3)	5(3)
C(5)	41(4)	46(4)	25(3)	4(3)	0(3)	-1(3)
C(6)	25(3)	20(3)	36(3)	4(2)	-4(3)	-10(2)
C(7)	25(3)	35(4)	30(3)	7(3)	-4(2)	4(3)
C(8)	45(5)	60(5)	49(4)	12(3)	-3(3)	20(4)
C(9)	48(5)	40(4)	43(4)	7(3)	-2(3)	8(3)
C(10)	64(6)	54(5)	95(6)	18(4)	-22(5)	1(4)
C(11)	110(9)	27(4)	125(8)	6(4)	-31(7)	3(5)
C(12)	114(9)	62(6)	90(7)	-10(5)	-25(6)	48(6)
C(13)	31(4)	46(4)	50(4)	13(3)	-1(3)	7(3)
C(14)	48(5)	72(5)	56(4)	12(4)	7(4)	-14(4)
C(15)	25(4)	33(3)	46(4)	3(3)	2(3)	-3(3)
C(16)	44(5)	48(4)	80(5)	11(4)	17(4)	4(3)
C(17)	50(6)	63(5)	126(8)	21(5)	14(5)	13(4)
C(18)	40(5)	73(6)	94(6)	18(5)	9(4)	17(4)
C(19)	31(4)	63(5)	56(4)	1(3)	6(3)	4(3)
C(20)	31(4)	44(4)	33(3)	2(3)	6(3)	-2(3)
C(21)	34(4)	48(4)	28(3)	6(3)	0(3)	-11(3)
C(22)	44(4)	46(4)	49(4)	9(3)	-2(3)	-17(3)
C(23)	72(6)	49(5)	67(5)	9(4)	8(4)	-32(4)
C(24)	75(6)	36(4)	81(6)	20(4)	-2(5)	-7(4)
C(25)	43(4)	46(4)	53(4)	10(3)	-8(3)	-3(3)
C(26)	27(4)	91(6)	76(5)	6(5)	5(4)	-13(4)
C(27)	44(5)	77(6)	69(5)	8(4)	7(4)	-32(4)
C(28)	75(6)	39(4)	42(4)	-1(3)	14(4)	-3(4)
C(29)	80(6)	56(5)	36(4)	13(3)	9(4)	14(4)
C(30)	63(5)	63(5)	33(4)	-8(3)	1(3)	16(4)
C(31)	34(4)	41(4)	43(4)	-8(3)	2(3)	7(3)
C(32)	22(3)	37(3)	38(3)	-7(3)	1(3)	4(3)
C(33)	23(3)	30(3)	42(3)	-7(3)	1(3)	-2(2)
C(34)	33(4)	35(4)	57(4)	-5(3)	10(3)	-1(3)
C(35)	48(4)	28(3)	74(5)	-5(3)	9(4)	-7(3)
C(36)	48(4)	40(4)	55(4)	10(3)	9(4)	3(3)
C(37)	35(4)	37(4)	39(3)	1(3)	10(3)	0(3)
C(38)	37(4)	65(5)	50(4)	-22(4)	-5(3)	0(3)
C(39)	39(4)	45(4)	64(5)	-22(4)	-2(3)	-8(3)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $Zn_2(phen)_4U_4O_{10}(OAc)_2(NA)_2(QA)_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	*U*(eq)
H(3)	6301	2404	-2162	80
H(4)	5854	2239	-665	80
H(5)	4352	2697	-176	80
H(8)	10516	3030	-3230	80
H(10)	8071	1867	-3144	80
H(11)	9129	979	-2830	80
H(12)	10845	1161	-2664	80
H(14A)	287	4945	-3762	80
H(14B)	1246	4719	-3158	80
H(14C)	762	4246	-3903	80
H(16)	1082	4953	-1166	80
H(17)	-657	5213	-1342	80
H(18)	-1847	4408	-1260	80
H(23)	-185	1374	-492	80
H(24)	1570	1213	-380	80
H(25)	2661	2095	-575	80
H(26)	-2262	3195	-998	80
H(27)	-1690	2170	-720	80
H(28)	2787	2965	1035	80
H(29)	3364	3270	2493	80
H(30)	3940	4329	2768	80
H(35)	4018	6343	-802	80
H(36)	3489	5929	-2186	80
H(37)	2886	4856	-2305	80
H(38)	4333	5451	2126	80
H(39)	4351	6144	911	80

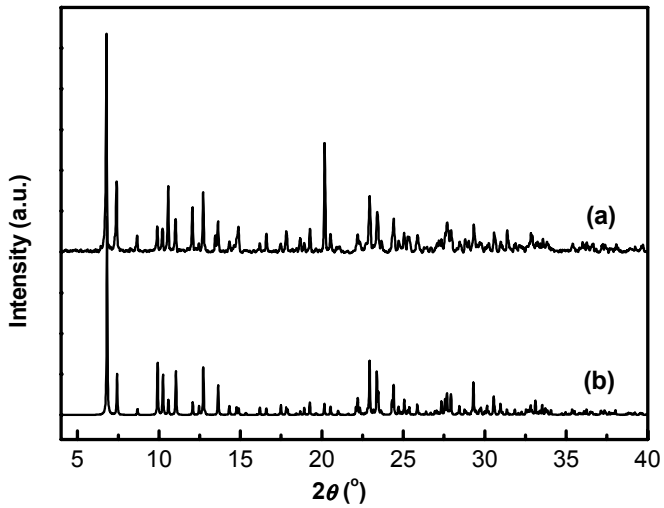

Figure S1. Comparison of the experimental XRD pattern (a) for **1** with the pattern simulated on the basis of the single crystal structure for **1** (b).

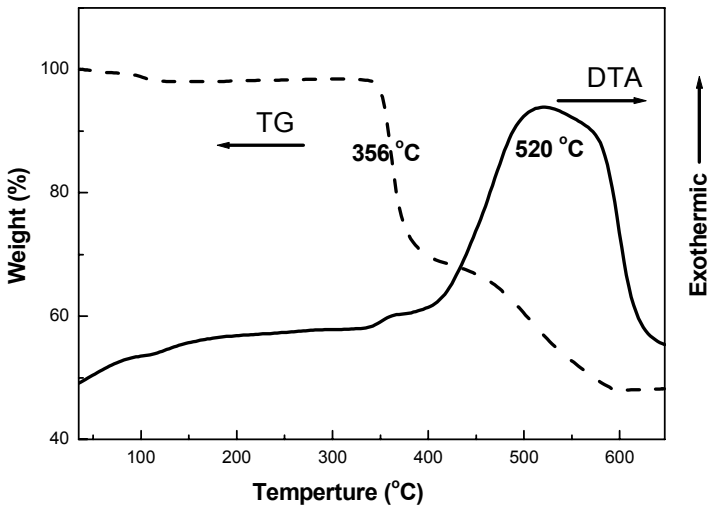

Figure S2. TG-DTA curves of **1**.

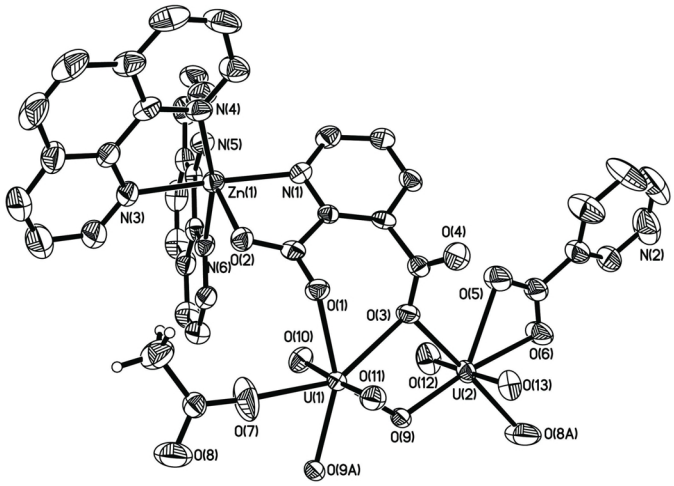

Figure S3. ORTEP drawing of the asymmetric unit of **1**. Thermal ellipsoids are shown at 50 % probability.

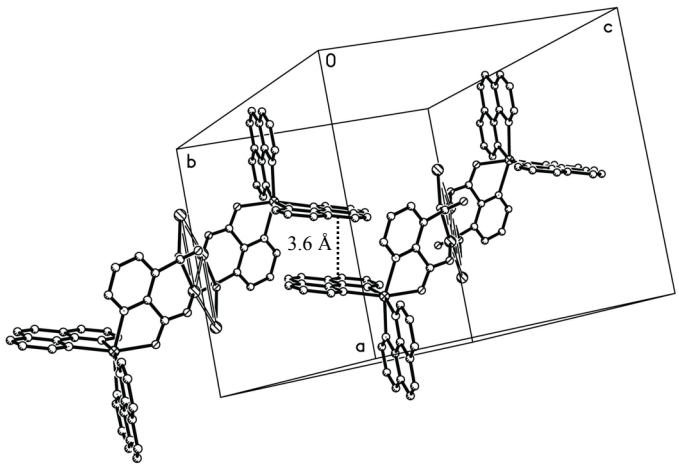

Figure S4. View of the compacted aromatic π-π stacking interaction between the adjacent two phen in **1**.

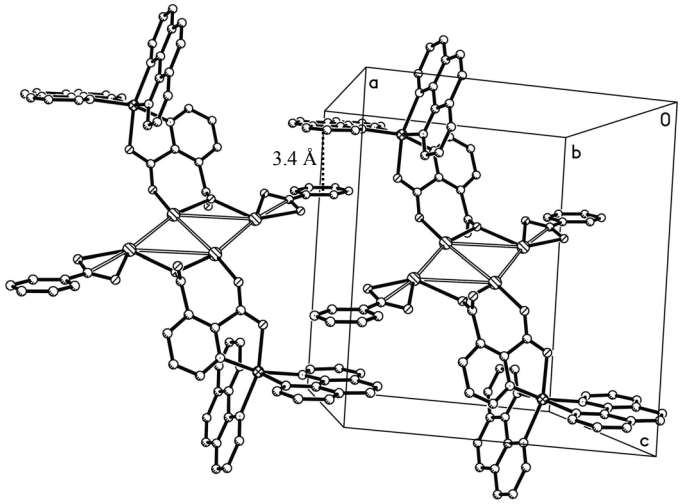

Figure S5. View of the aromatic π-π stacking interaction between the adjacent phen and the NA ligand in **1**.

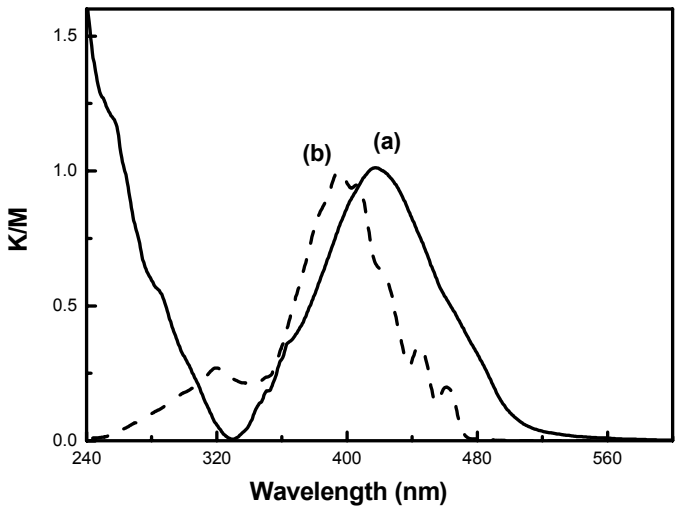

Figure S6. (a) UV-vis diffuse reflectance spectrum of **1** using $BaSO_4$ as the background, and for comparison, the spectrum of $UO_2(OAc)_2 \cdot 2H_2O$ (b) is also shown.

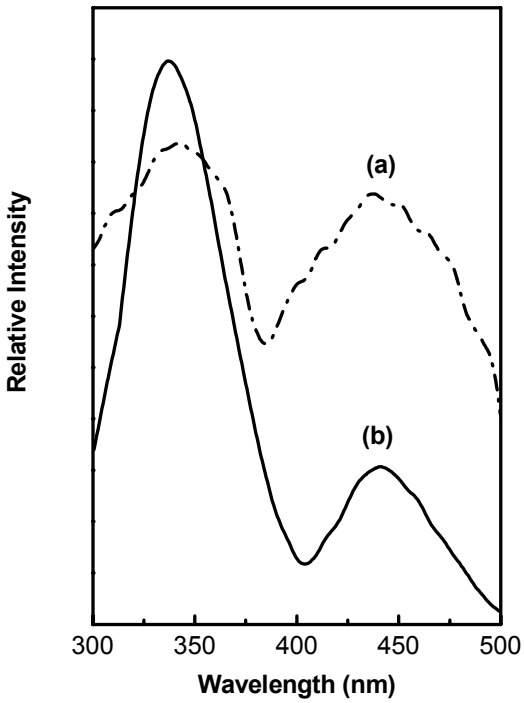

Figure S7. Comparison of the excitation spectrum (a) and the SPS (b) for **1**.

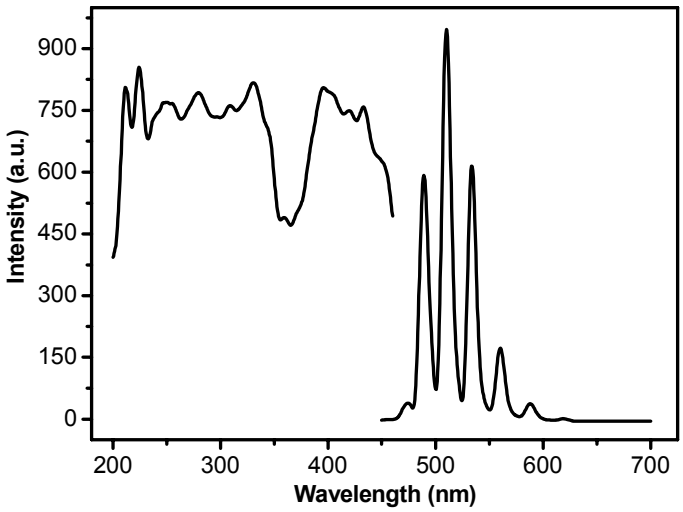

Figure S8. Excitation spectrum (left) and solid state emission spectrum (right) for $UO_2(OAc)_2 \cdot 2H_2O$ at room temperature.