Formation of Uranyl Phthalate Coordination Polymers with Unusual 2D Net Topologies in the Presence of Organic Cations

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Supporting Information

Table S1. Main Interatomic Distances (Å) in the Structure of $(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$

U1-O1	1.758(4)	U2-O10	1.768(4)
U1-O1	1.758(4)	U2-O11	1.773(4)
U1-O6	2.362(4)	U2-O8	2.281(4)
U1-O6	2.362(4)	U2-O3	2.379(4)
U1-O4	2.513(4)	U2-O2	2.394(4)
U1-O4	2.513(4)	U2-O7	2.406(4)
U1-O5	2.623(4)	U2-O5	2.500(4)
U1-O5	2.623(4)		

Table S2. Main Interatomic Distances (Å) in the Structure of $(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$

U1-O1	1.762(5)	U2-O3	1.765(5)	U3-O4	1.761(4)	U4-O6	1.755(4)
U1-O2	1.761(5)	U2-O18	2.306(4)	U3-O5	1.773(4)	U4-O7	1.759(4)
U1-O10	2.355(4)	U2-O24	2.246(5)	U3-O12	2.428(4)	U4-O9	2.437(4)
U1-O11	2.328(4)			U3-O17	2.381(4)	U4-O14	2.411(4)
U1-O13	2.406(4)			U3-O19	2.474(4)	U4-O15	2.456(5)
U1-O16	2.380(4)			U3-O21	2.287(4)	U4-O25	2.365(4)
U1-O20	2.370(4)			U3-O23	2.390(4)	U4-O25’	2.366(4)

Table S3. Main Interatomic Distances (Å) in the Structure of (*t*-$BuNH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$

U1-O1	1.786(4)	U2-O3	1.756(4)
U1-O2	1.782(4)	U2-O4	1.784(4)
U1-O5	2.581(4)	U2-O5	2.422(4)
U1-O6	2.555(4)	U2-O8	2.355(4)
U1-O9	2.617(4)	U2-O9	2.433(4)
U1-O10	2.564(4)	U2-O12	2.325(4)
U1-O13	2.252(4)	U2-O13	2.200(4)
U1-O13’	2.270(4)		

Table S4. Main Interatomic Distances (Å) in the Structure of $(C_2H_5NH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$

U1-O1	1.760(7)	U2-O3	1.776(7)
U1-O2	1.761(7)	U2-O4	1.755(7)
U1-O5	2.608(5)	U2-O5	2.424(5)
U1-O6	2.543(5)	U2-O8	2.352(5)
U1-O9	2.614(5)	U2-O9	2.423(5)
U1-O10	2.555(6)	U2-O12	2.343(5)
U1-O13	2.248(5)	U2-O13	2.185(5)
U1-O13’	2.263(5)		

Table S5. Main Interatomic Distances (Å) in the Structure of $\{As(C_6H_5)_4\}_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot 8H_2O$

U1-O1	1.768(4)	U2-O3	1.761(4)
U1-O2	1.790(4)	U2-O4	1.783(4)
U1-O5	2.636(4)	U2-O5	2.463(4)
U1-O6	2.567(4)	U2-O8	2.320(4)
U1-O9	2.576(4)	U2-O9	2.429(4)
U1-O10	2.570(4)	U2-O12	2.324(4)

U1-O13	2.244(4)	U2-O13	2.220(4)
U1-O13’	2.255(4)		

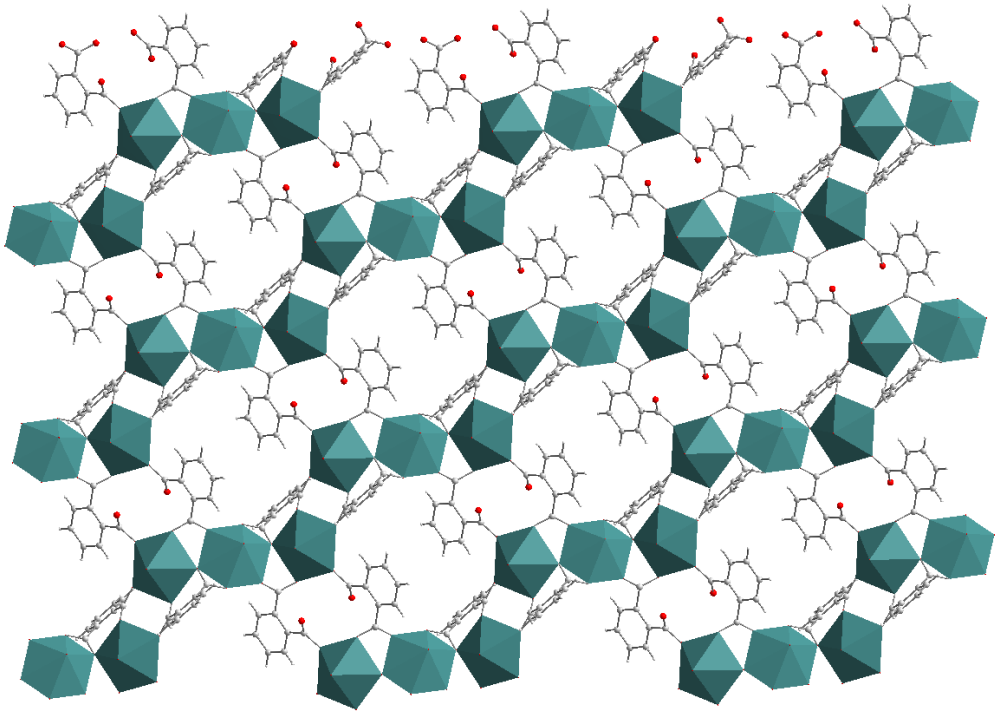

Figure S1. Polyhedral representation of the layer in the structure of $(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$

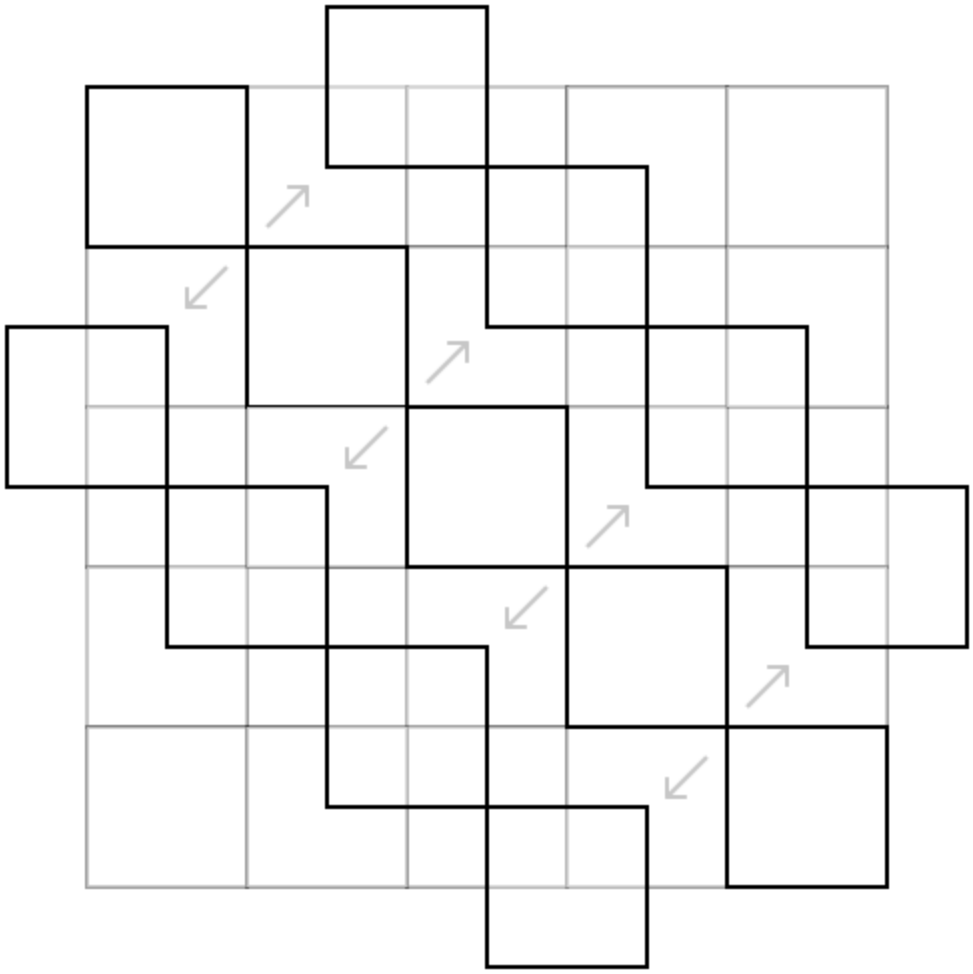

Figure S2. Transformation of the *sql* to the $(4.8.4.8)(4^3.8)_2(4^2.8)_4$ topology

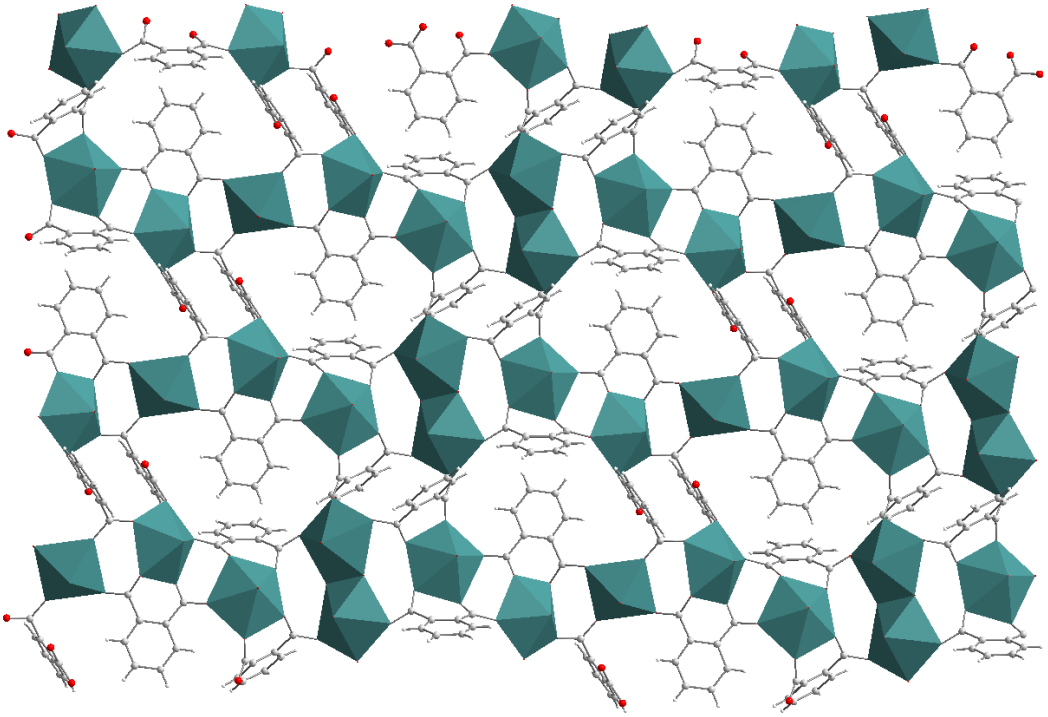

Figure S3. Polyhedral representation of the layer in the structure of $(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$

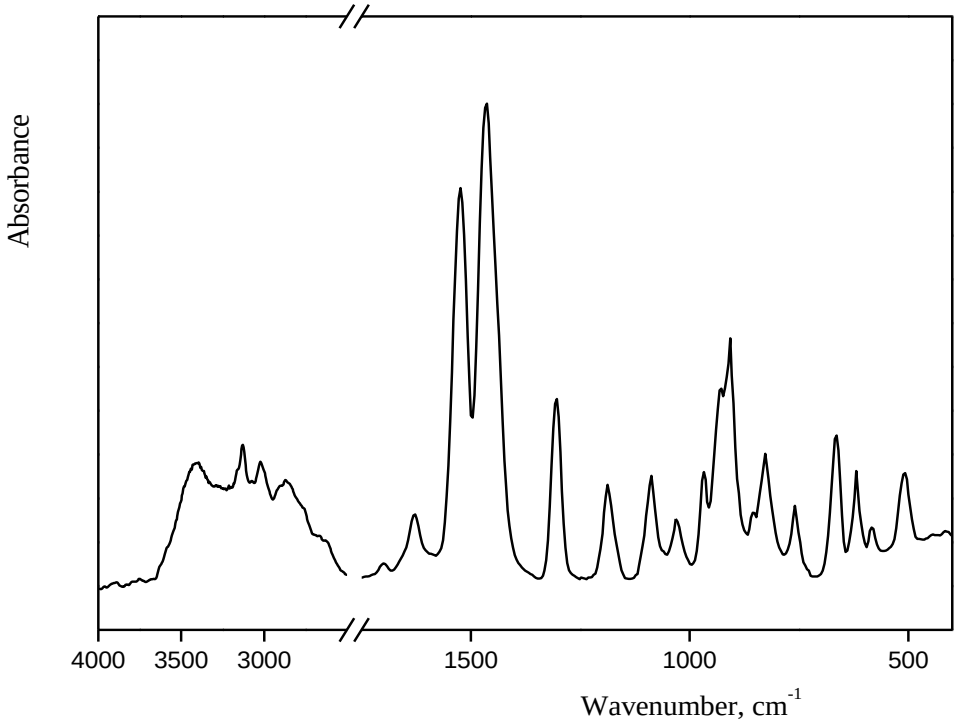

Figure S4. Infrared spectrum of $(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$

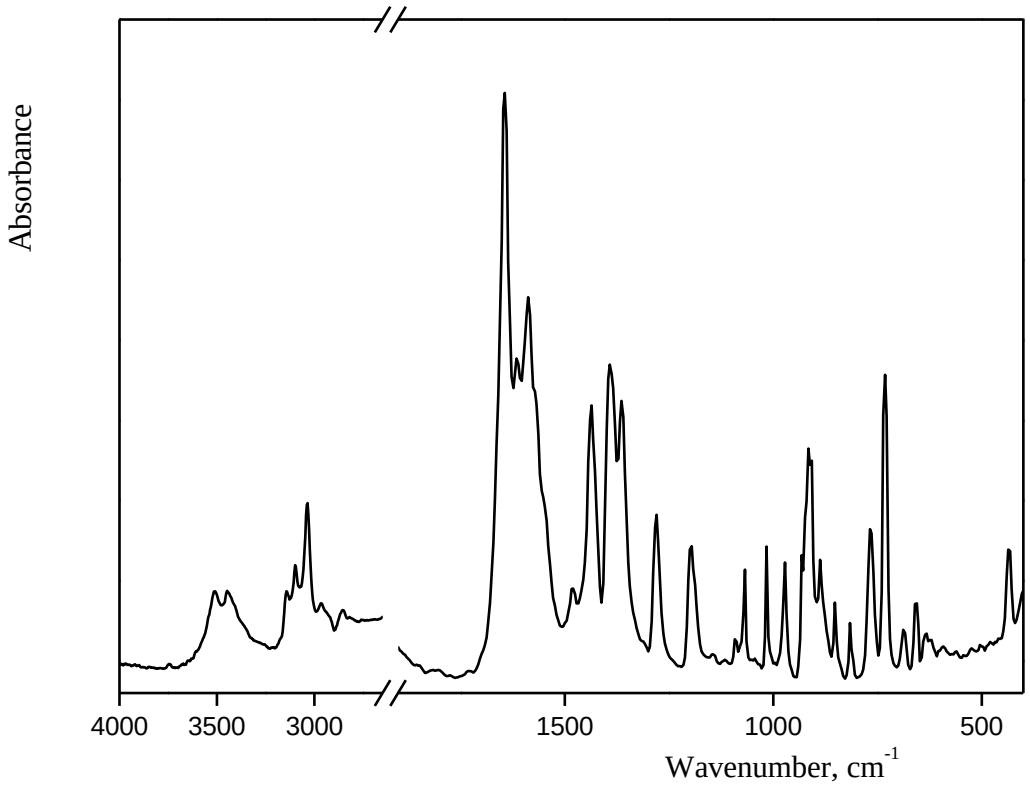

Figure S5. Infrared spectrum of $(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$

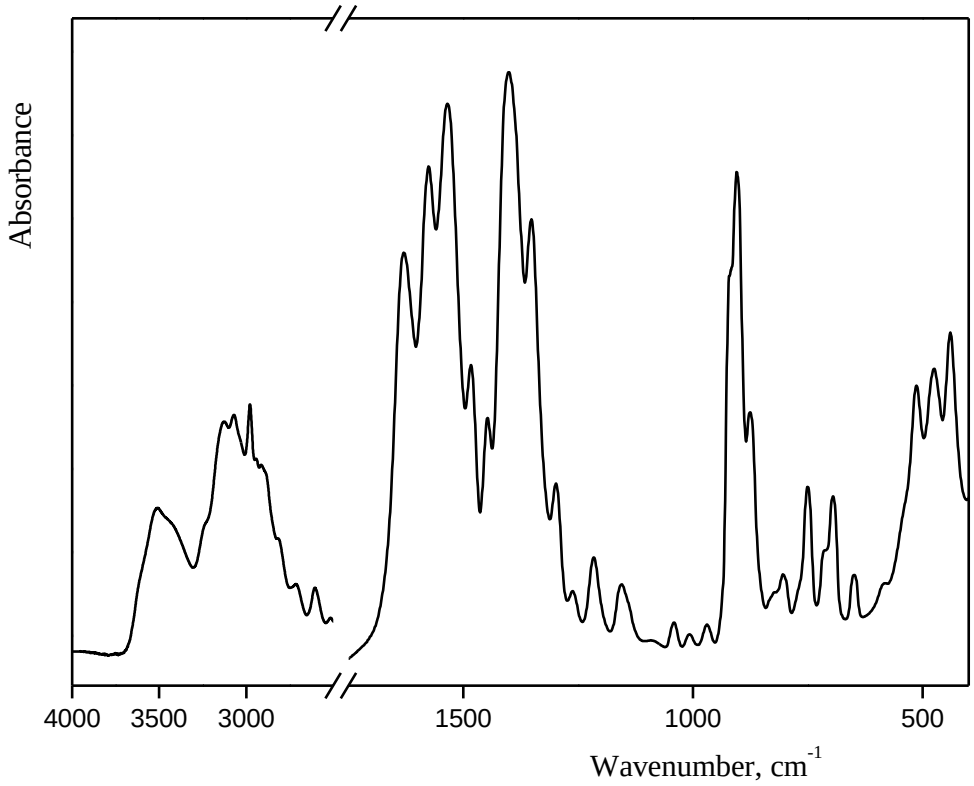

Figure S6. Infrared spectrum of (*t*-$BuNH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$

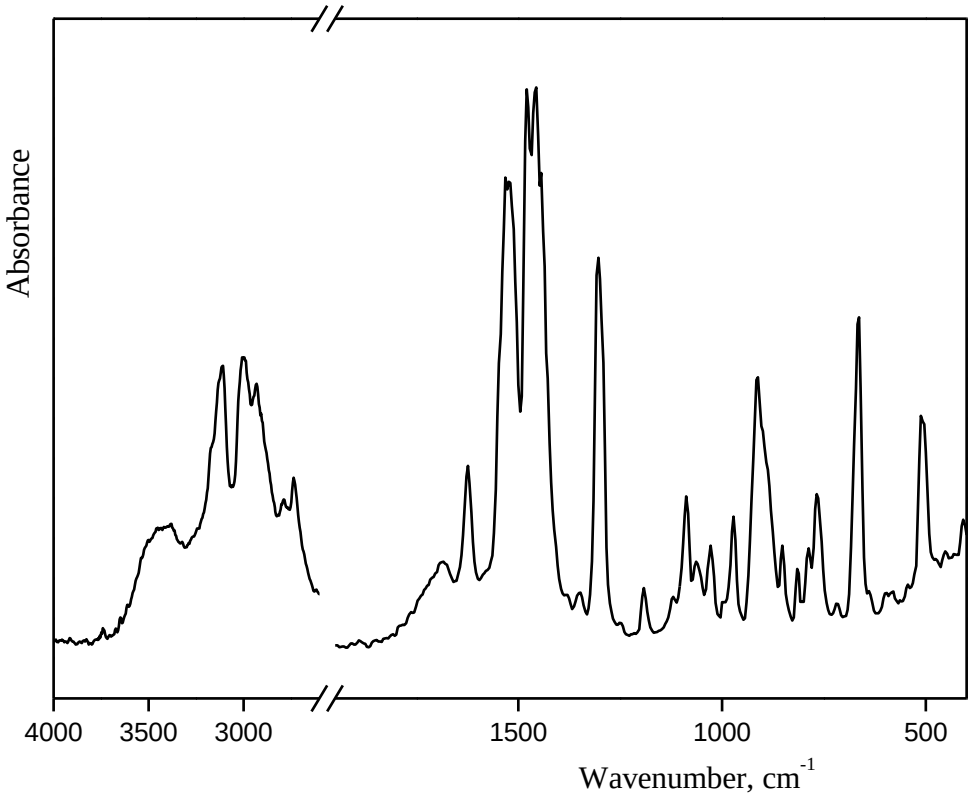

Figure S7. Infrared spectrum of $(C_2H_5NH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$

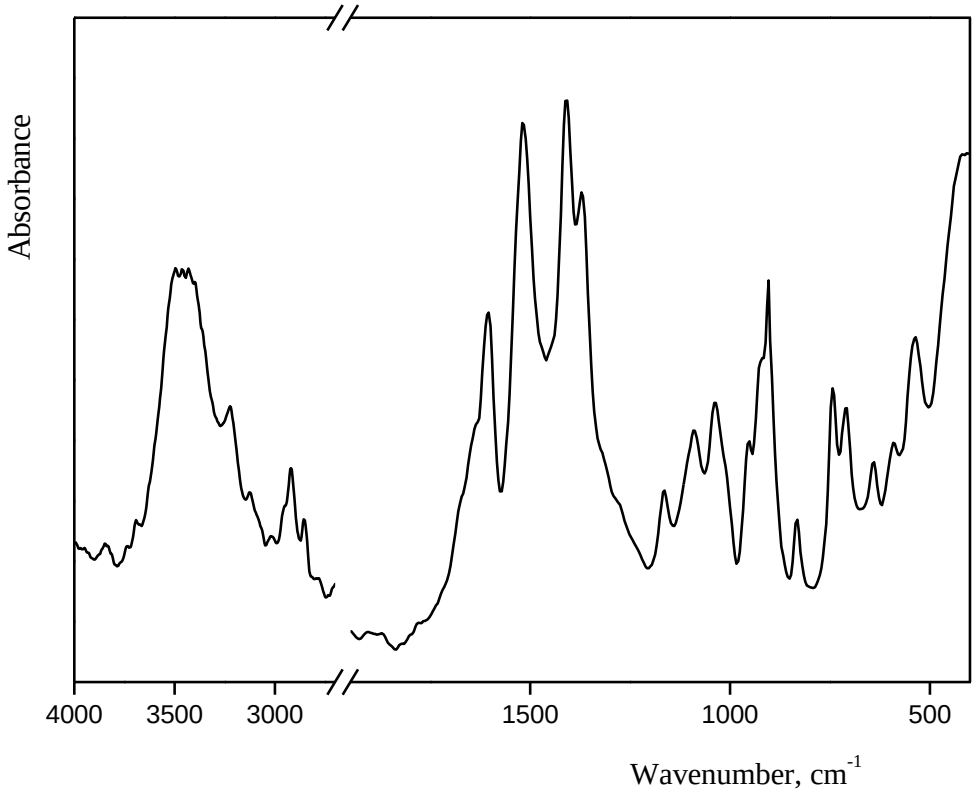

Figure S8. Infrared spectrum of $\{As(C_6H_5)_4\}_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot 8H_2O$

Table S6. Vibrational frequencies and their assignments in IR spectra

Complex	Frequency, cm^{-1}
$(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$	3506, 3402, 3350, 3268, 3199, 3132, 3074, 3022- ν(OH), $\nu(NH)_{imid}$; 2928, 2866, 2782, 2654 - ν(CH); 1628 - $\delta(H_2O)$; 1522, 1464 - ν(C-C), ν(C-N), ν(CCO), 1304 - δ(CH); 1189, 1088, 1062, 1030 - δ(CC), δ(CH); 928/ 914 - $\nu(UO_2)$; 854, 826, 760 - δ_{ip} $(CH)_{ring}$, δ_{oop} $(NH)_{imid}$, , 664 – δ_{oop} $(CC)_{ring}$; 620, 583, 509 - δ(CH), δ(CC) 446 – ρ(OCO)
$(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$	3516, 3442 - ν(OH); 3144 3103; 3045 - $\nu(NH)_{imid}$; 2962, 2918, 2882, 2864 - ν(CH), $\nu(CH_3)$; 1612; 1587; 1484; 1424; 1388 - ν(C-C), ν(C-N), ν(CCO); 1362; 1282; 1198; 1146; 1090; 1068; 1014 - δ(CC), δ(CH), $\delta(CH_3)$; 972 γ(CH); 928/ 914/ 904 - $\nu(UO_2)$;; 888; 854; 820 - 768; 732 - ρ(CH); δ_{ip} $(CH)_{ring}$, δ_{oop} $(NH)_{imid}$; 690; 628 - δ(CH), δ(CC), δ(OH); 432 - γ(OH)
$(t\text{-}BuNH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$	3514, 3416 - ν(OH); 3178; 3145 - ν(NH); 2996; 2918; 2828; 2712 - ν(CH), $\nu(CH_3)$; 1638, 1619, 1579, 1535, 1481 - $\delta(H_2O)$, ν(C-C), δ(NH), ν(CCO); 1438; 1412; 1350 - $\delta(CH_3)$; 1237 – $\nu(C_3C\text{-}N)$; 1110; 1050; 948 - δ(CC), δ(CH), $\delta(CH_3)$; 924/ 908 - $\nu(UO_2)$; 870, 818 - γ(CH); δ_{ip} $(CH)_{ring}$; 764; 652; 542 – $\rho/\omega(H_2O)$
$(C_2H_5NH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$	3464; 3380 - ν(OH); 3160, 3112 - ν(NH);; 2998; 2933; 2796; 2736 - ν(CH), $\nu(CH_3)$;; 1624; 1532/ 1520; 1480; 1460 - $\delta(H_2O)$, ν(C-C), δ(NH), ν(CCO);; 1351, 1303 $\delta(CH_3)$; 1192; 1087; 1063; 1028 - δ(CH), δ(CC); 971 - γ(CH); 922/ 904 - $\nu(UO_2)$; 860; 820 - ρ(CH), δ_{ip} $(CH)_{ring}$; 785; 766; 718 - γ(CH) , 664; 510 – $\rho/\omega(H_2O)$
$\{As(C_6H_5)_4\}_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot 8H_2O$	3502, 3460, 3496, 3432, 3225 - ν(OH);; 3020; 2956; 2918; 2850, 2772 - ν(CH); 1670sh, 1630sh, 1609; 1515 - $\delta(H_2O)$, ν(C-C), δ(NH), ν(CCO); 1410; 1372 - δ(CH); 1165; 1092; 1036; 952sh - δ(CH), δ(CC); γ(CH);; 926/ 912 - $\nu(UO_2)$; 834 - γ(CH); 743; 708 - $\delta(CCC)_{ring}$; 644; 592; 538 – $\rho/\omega(H_2O)$

Table S7. The characteristics of UV-VIS spectra of compounds

Complex	*The main peak positions, cm^{-1}
$(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$	24429, 24166, 23820, 23568, **22967**, 22291, 22119
$(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$	26413, 25100, 24479, 23758, **23062**, 22326, 21593, 20185
$(t\text{-}BuNH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$	26831, 25967, 24777, 24148, **23452**, 22914, 22084, 21321, 20656, 19692, 15951
$(C_2H_5NH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$	27070, 26406, 24950, 24242, **23579**, 22972, 22197, 20837, 19376, 18491, 17044
$\{As(C_6H_5)_4\}_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot 8H_2O$	24521, **23546**, 22737, 21123, 19493, 18261, 16940

*highlighted major peaks

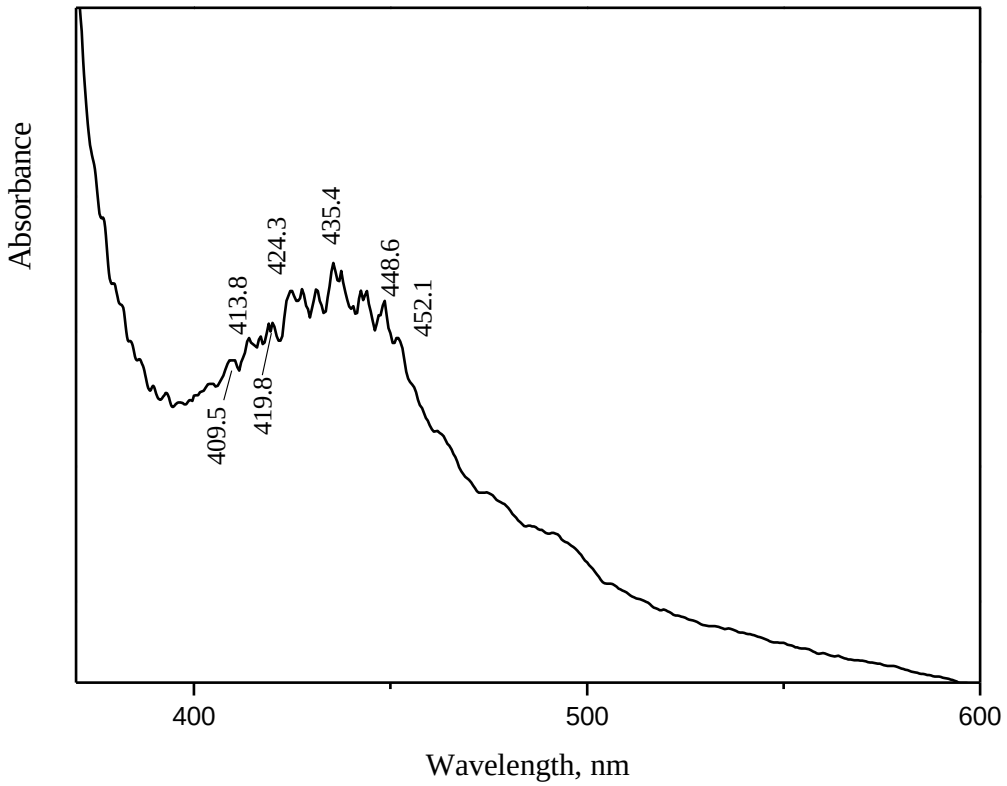

Figure S9. UV-VIS spectrum of $(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$

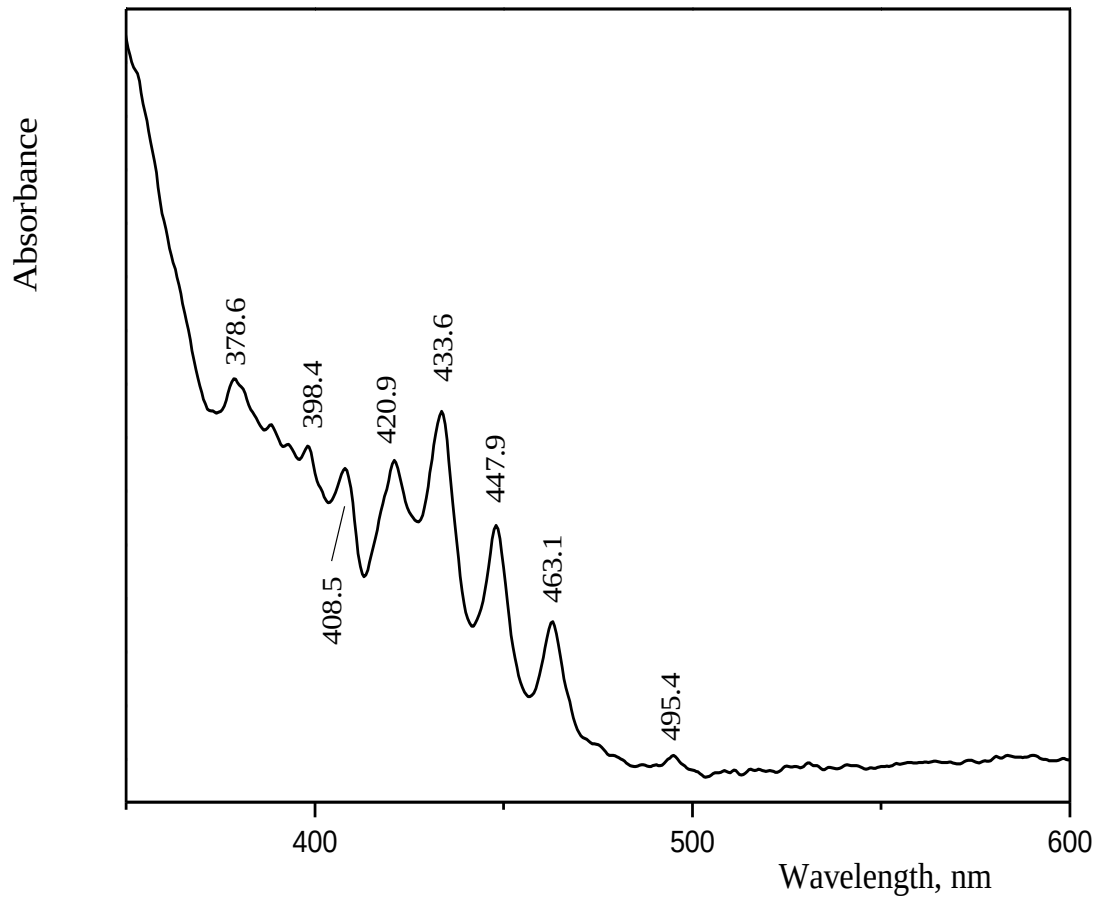

Figure S10. UV-VIS spectrum of $(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$

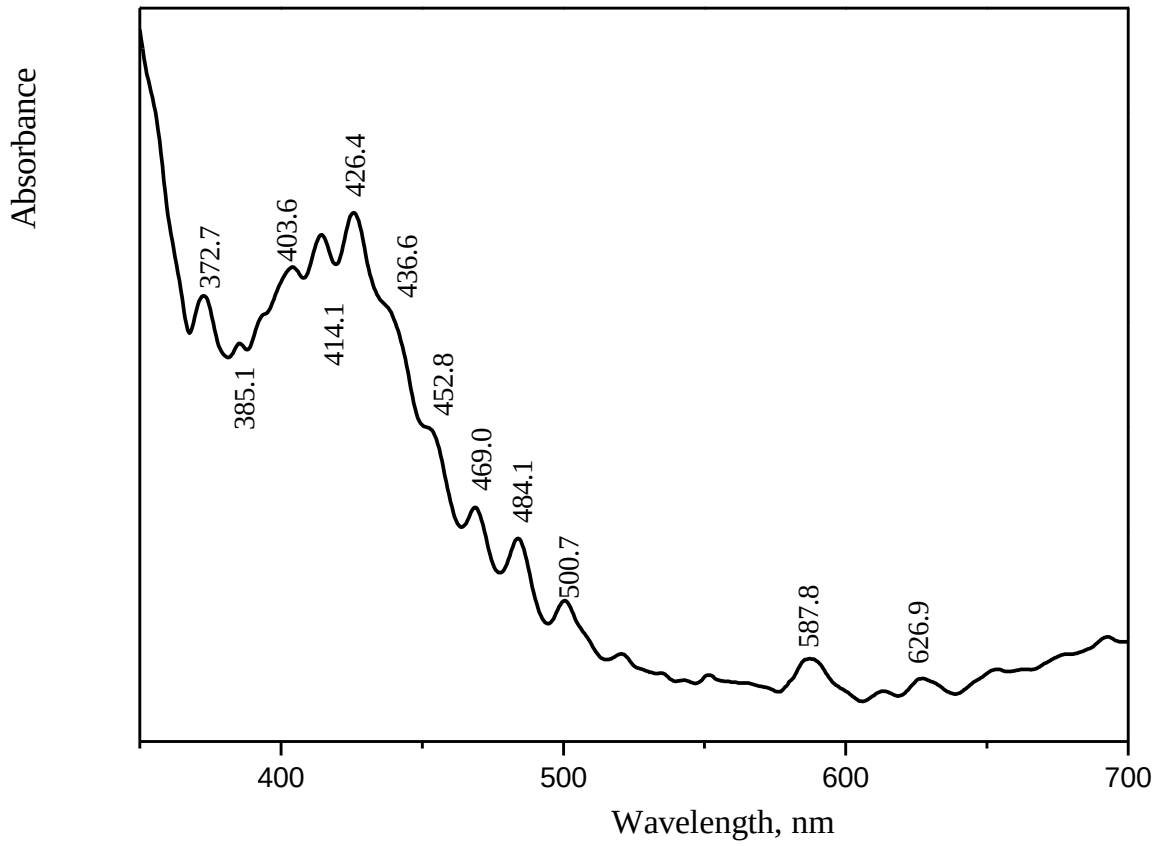

Figure S11. UV-VIS spectrum of (*t*-$BuNH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$

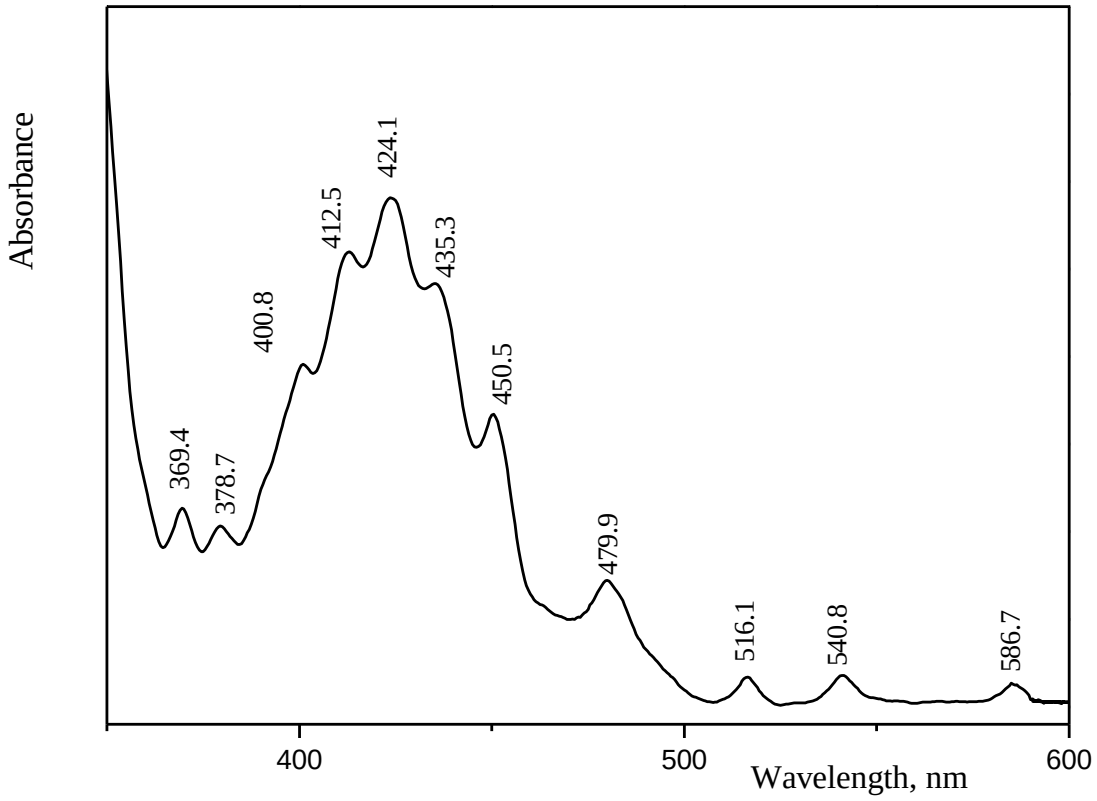

Figure S12. UV-VIS spectrum of $(C_2H_5NH_3)_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot nH_2O$

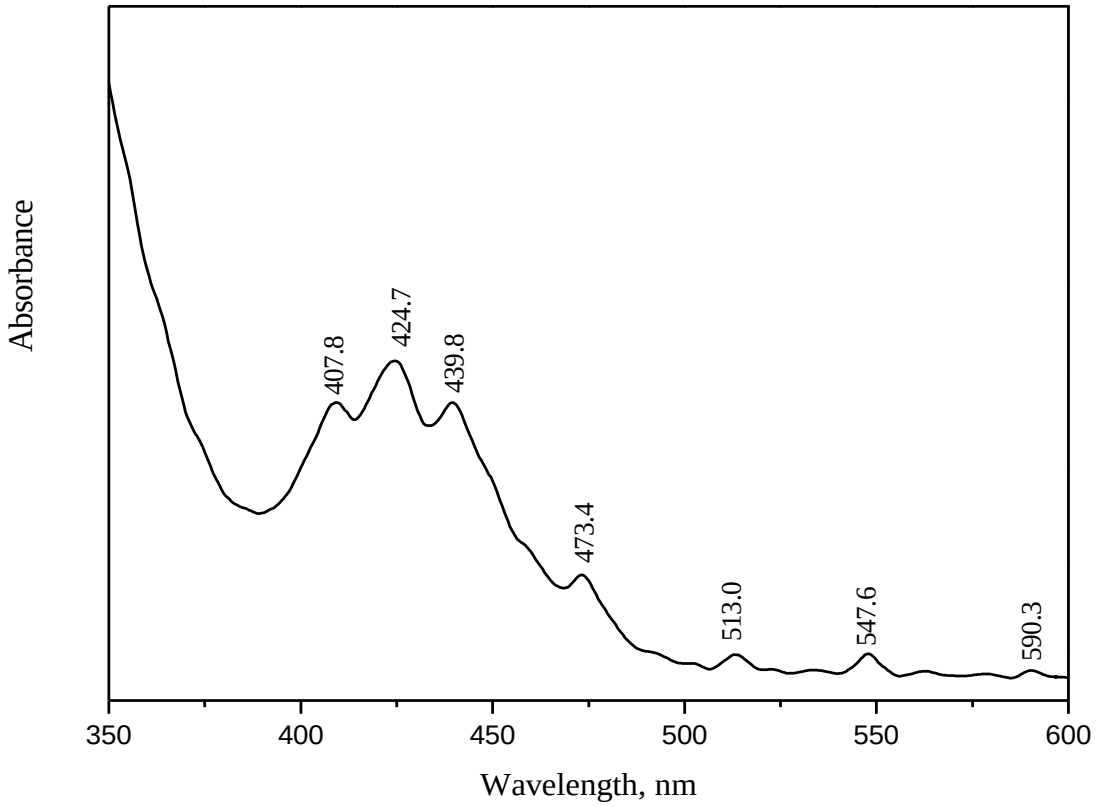

Figure S13. UV-VIS spectrum of $\{As(C_6H_5)_4\}_4[(UO_2)_4(O)_2\{C_6H_4(COO)_2\}_4]\cdot 8H_2O$

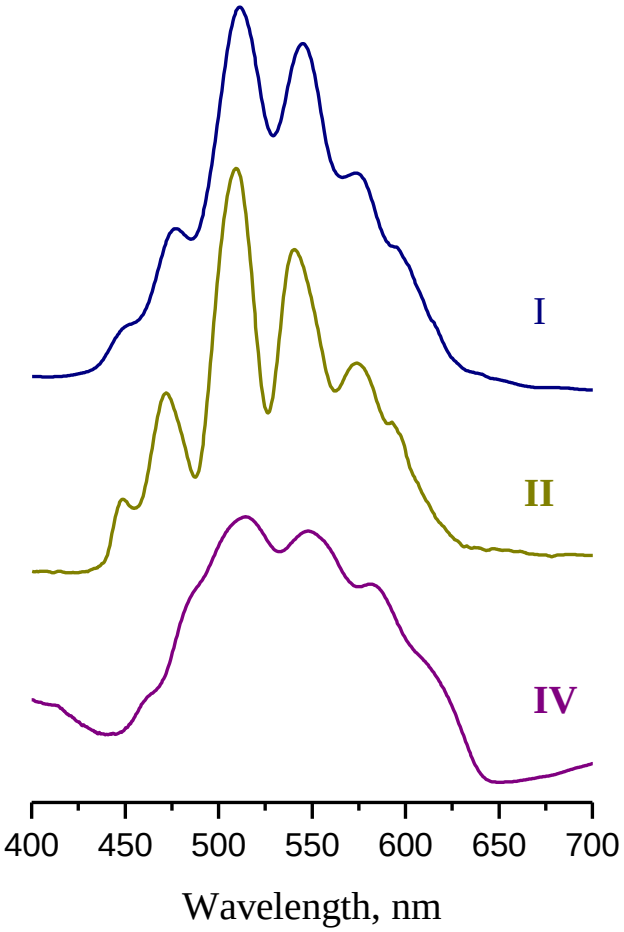

Figure S14. The luminescence spectra of solid compounds **1**, **2**, and **4**

Table S8. The data of the thermal analysis of solid compounds **1**, **2**, and **4**

Complex	Stage	ΔT °C	Δm, %	
			Calc.	Found
$(Him)_2[(UO_2)_3\{C_6H_4(COO)_2\}_4]\cdot 2H_2O$	I	75 – 110	2.2	1.70
(m_i = 39.815 mg)	II	200 – 300	8.42	8.84
	III	300 – 600	40.02	40.82
	$UO_2 \rightarrow U_3O_8$	> 600		
$(HMeIm)_4[(UO_2)_7\{C_6H_4(COO)_2\}_8(OH)_2]$	I	190 -360	10.26	10.06
(m_i = 22.411 mg)	II	420 -530	36.78	37.05
	$UO_2 \rightarrow U_3O_8$	> 600		
$(C_2H_5NH_3)_4[(UO_2)_4(C_8H_4O_4)_4(O)_2]\cdot nH_2O$	I	90 – 160	26.77	27.05
(m_i = 21.718 mg)	II	300 – 450	25.41	26.02
	III	450 – 600	13.6	13.75
	$UO_2 \rightarrow U_3O_8$	> 600		