Supplementary Material

Uranyl-containing heterometallic coordination polymers based on 4-(4'-carboxyphenyl)-1,2,4-triazole ligand: Structure regulation through subtle changes of the secondary metal centers

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Table S1. Selected Bond Lengths (Å) and Bond Angles **(°)** for **1**.

Bond	Dist.	Bond	Dist.
U1-O1	1.7824(19)	Cd1-N2	2.360(2)
U1-O3	2.4090(18)	Cd1-N2^{ii}	2.360(2)
U1-O2	1.766(2)	Cd1-N5^{ii}	2.281(2)
U1-O4	2.4905(17)	Cd1-N5	2.281(2)
U1-O5^{i}	2.5204(17)	Cd1-O9W^{ii}	2.3749(19)
U1-O6^{i}	2.4410(18)	Cd1-O9W	2.3749(19)
U1-O7	2.4788(18)		
U1-O8	2.4838(17)		
Angle	(°)		
O1-U1-O3	90.07(8)	Angle	(°)
O1-U1-O4	89.03(7)	N2-Cd1-N2^{ii}	92.92(10)
O1-U1-O5^{i}	89.43(7)	N2-Cd1-O9W	82.57(7)
O1-U1-O6^{i}	90.91(8)	N2-Cd1-O9W^{ii}	81.25(7)
O1-U1-O7	87.20(8)	N2^{ii}-Cd1-O9W^{ii}	82.57(7)
O1-U1-O8	90.59(7)	N2^{ii}-Cd1-O9W	81.25(7)
O3-U1-O4	53.15(6)	N5-Cd1-N2	87.17(7)
O3-U1-O5^{i}	116.07(6)	N5^{ii}-Cd1-N2	175.67(8)
O3-U1-O6^{i}	63.88(6)	N5^{ii}-Cd1-N2^{ii}	87.17(7)
O3-U1-O7	175.64(6)	N5-Cd1-N2^{ii}	175.66(8)
O3-U1-O8	124.02(6)	N5^{ii}-Cd1-N5	93.06(10)
O2-U1-O1	178.21(9)	N5-Cd1-O9W^{ii}	101.72(7)
O2-U1-O3	91.60(8)	N5^{ii}-Cd1-O9W	101.72(7)
O2-U1-O4	91.45(8)	N5^{ii}-Cd1-O9W^{ii}	94.47(7)
O2-U1-O5^{i}	90.42(8)	N5-Cd1-O9W	94.47(7)
O2-U1-O6^{i}	90.40(8)	O9W-Cd1-O9W^{ii}	156.42(9)
O2-U1-O7	91.09(8)		
O2-U1-O8	87.94(8)		
O4-U1-O5^{i}	169.11(6)		
O6^{i}-U1-O4	117.03(6)		
O6^{i}-U1-O5^{i}	52.21(6)		
O6^{i}-U1-O7	119.53(6)		
O6^{i}-U1-O8	171.95(6)		
O7-U1-O4	123.34(6)		
O7-U1-O5^{i}	67.33(6)		
O7-U1-O8	52.66(5)		
O8-U1-O4	70.90(6)		
O8-U1-O5^{i}	119.90(6)		

Symmetry transformation: (i) 0.5-x, -0.5+y, 1.5-z; (ii) 1-x, y, 0.5-z.

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) for **2**.

Bond	Dist.	Bond	Dist.
U1-O1	1.774(2)	Zn1-N3^{ii}	2.157(2)
U1-O2	1.760(2)	Zn1-N3	2.157(2)
U1-O3	2.479(2)	Zn1-N6^{ii}	2.094(2)
U1-O4	2.427(2)	Zn1-N6	2.094(2)
U1-O5^{i}	2.4875(19)	Zn1-O9W	2.1870(19)
U1-O6^{i}	2.4808(18)	Zn1-O9W^{ii}	2.1870(19)
U1-O7	2.4741(17)		
U1-O8	2.4699(18)		
Angle	(°)	Angle	(°)
O1-U1-O3	90.47(10)	N3-Zn1-N3^{ii}	180.000
O1-U1-O4	93.68(11)	N3^{ii}-Zn1-O9W	97.60(8)
O1-U1-O5^{i}	89.55(9)	N3-Zn1-O9W	82.40(8)
O1-U1-O6^{i}	87.54(9)	N3^{ii}-Zn1-O9W^{ii}	82.40(8)
O1-U1-O7	89.25(8)	N3-Zn1-O9W^{ii}	97.60(8)
O1-U1-O8	88.70(9)	N6-Zn1-N3^{ii}	92.48(8)
O2-U1-O1	178.07(10)	N6^{ii}-Zn1-N3	92.48(8)
O2-U1-O3	91.22(10)	N6^{ii}-Zn1-N3^{ii}	87.52(8)
O2-U1-O4	88.09(11)	N6-Zn1-N3	87.52(8)
O2-U1-O5^{i}	90.45(10)	N6-Zn1-N6^{ii}	180.00(12)
O2-U1-O6^{i}	90.94(9)	N6^{ii}-Zn1-O9W	90.46(8)
O2-U1-O7	90.48(9)	N6-Zn1-O9W	89.54(8)
O2-U1-O8	89.62(9)	N6^{ii}-Zn1-O9W^{ii}	89.54(8)
O3-U1-O5^{i}	118.97(7)	N6-Zn1-O9W^{ii}	90.46(8)
O3-U1-O6^{i}	170.68(6)	O9W-Zn1-O9W^{ii}	180.000
O4-U1-O3	52.74(7)		
O4-U1-O5^{i}	66.36(7)		
O4-U1-O6^{i}	118.29(7)		
O4-U1-O7	121.62(7)		
O4-U1-O8	173.74(7)		
O6^{i}-U1-O5^{i}	51.95(6)		
O7-U1-O3	68.96(6)		
O7-U1-O5^{i}	172.00(6)		
O7-U1-O6^{i}	120.09(6)		
O8-U1-O3	121.52(6)		
O8-U1-O5^{i}	119.50(6)		
O8-U1-O6^{i}	67.56(6)		
O8-U1-O7	52.56(6)		

Symmetry transformation: (i) -x, 2-y, 1-z; (ii) 1-x, 1-y, 2-z.

Table S3. Selected Bond Lengths (Å) and Bond Angles **(°)** for **3**.

Bond	Dist.
U1-O1	1.7854(17)
U1-O2	1.7818(17)
U1-O4	2.3408(17)
U1-N3^{ii}	2.5623(19)
U1-O3^{i}	2.3468(17)
U1-O3	2.3412(17)
U1-O5^{iii}	2.4085(16)

Angle	(°)
O1-U1-O4	89.31(7)
O1-U1-N3^{ii}	89.99(7)
O1-U1-O3	91.53(7)
O1-U1-O3^{i}	88.33(7)
O1-U1-O5^{iii}	83.56(7)
O2-U1-O1	174.87(7)
O2-U1-O4	90.35(7)
O2-U1-N3^{ii}	87.69(7)
O2-U1-O3^{i}	95.22(7)
O2-U1-O3	93.35(7)
O2-U1-O5^{iii}	91.35(7)
O4-U1-N3^{ii}	149.34(6)
O4-U1-O3	75.99(6)
O4-U1-O3^{i}	139.85(6)
O4-U1-O5^{iii}	79.09(5)
O3-U1-N3^{ii}	134.67(6)
O3^{i}-U1-N3^{ii}	70.75(6)
O3-U1-O3^{i}	64.02(7)
O3-U1-O5^{iii}	154.66(6)
O3^{i}-U1-O5^{iii}	140.22(6)
O5^{iii}-U1-N3^{ii}	70.37(6)

Symmetry transformation: (i) 2-x, 2-y, 1-z; (ii) x, 1+y, z; (iii) 1-x, 2-y, 1-z.

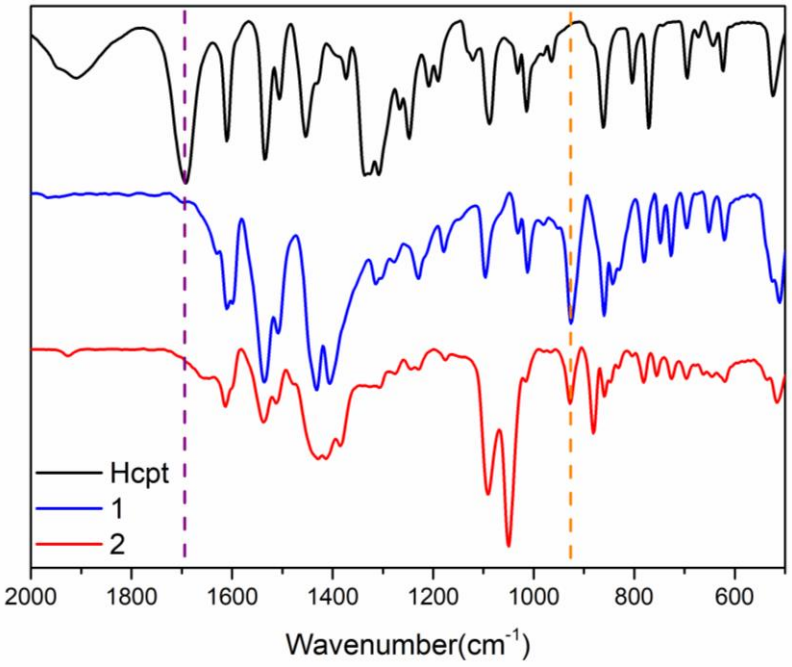

Figure S1. IR spectra for Hcpt(black), **1**(blue), and **2**(red). The peaks around 925 cm^{-1} (orange dash line) which can be attributed to the signal of $\nu(UO_2^{2+})$ show the presence of uranyl ions in **1** and **2**. The absence of characteristic absorption bands around 1730–1690 cm^{-1} (purple dash line) indicates that the carboxylate groups are completely coordinated to the metal centers in **1** and **2**.

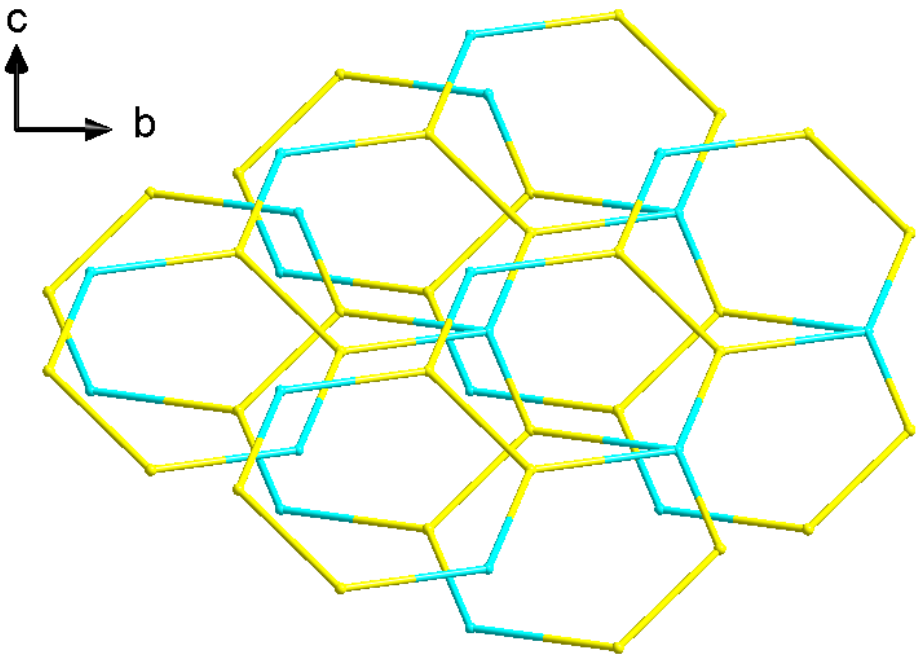

Figure S2. The overall topology representation of **1**.

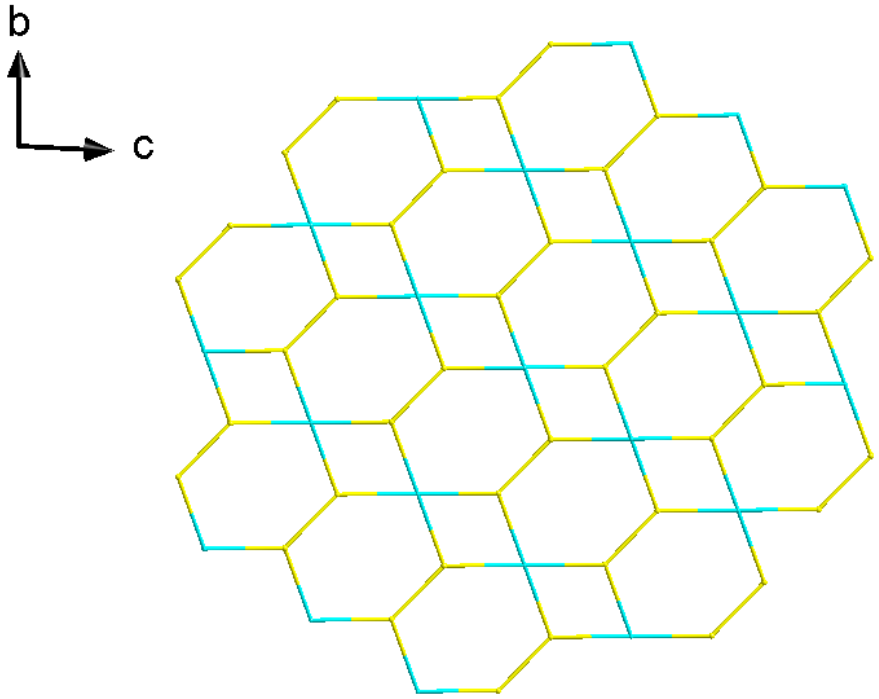

Figure S3. The overall topology representation of **2**.

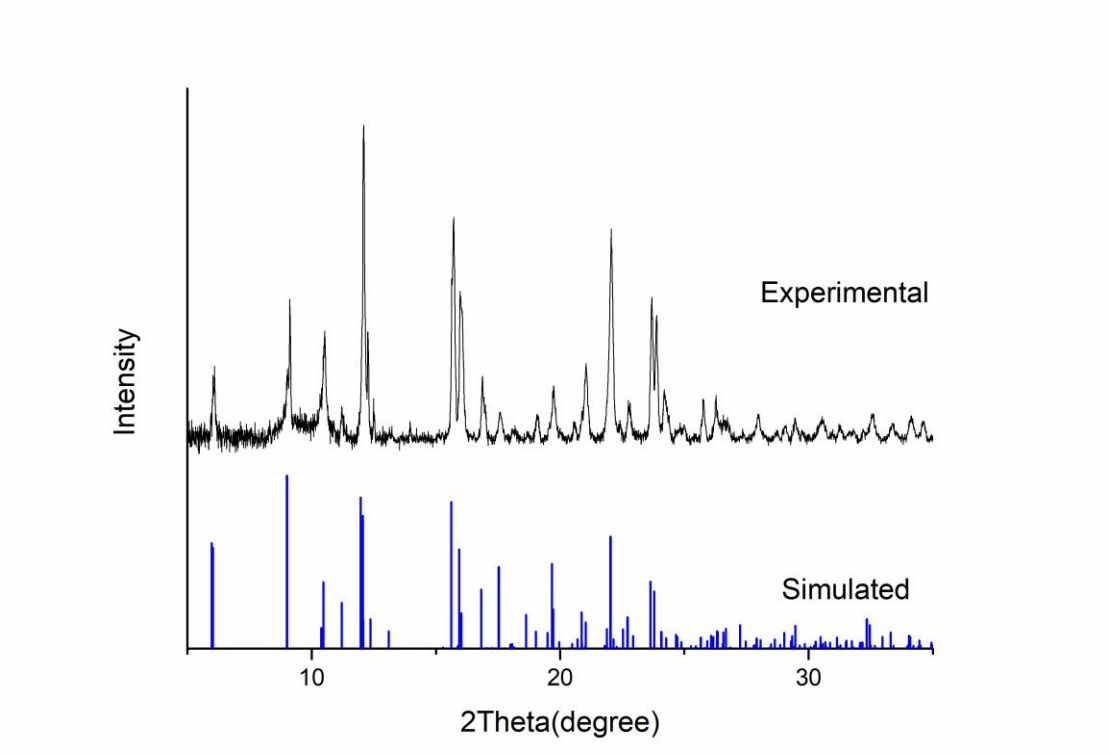

Figure S4. Simulated and experimental PXRD patterns for **1**.

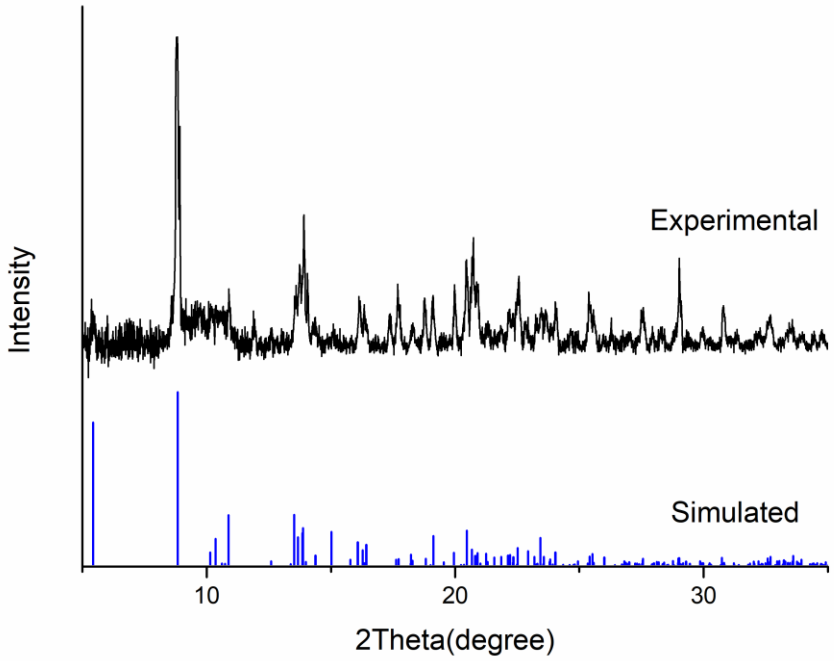

Figure S5. Simulated and experimental PXRD patterns for **2**.

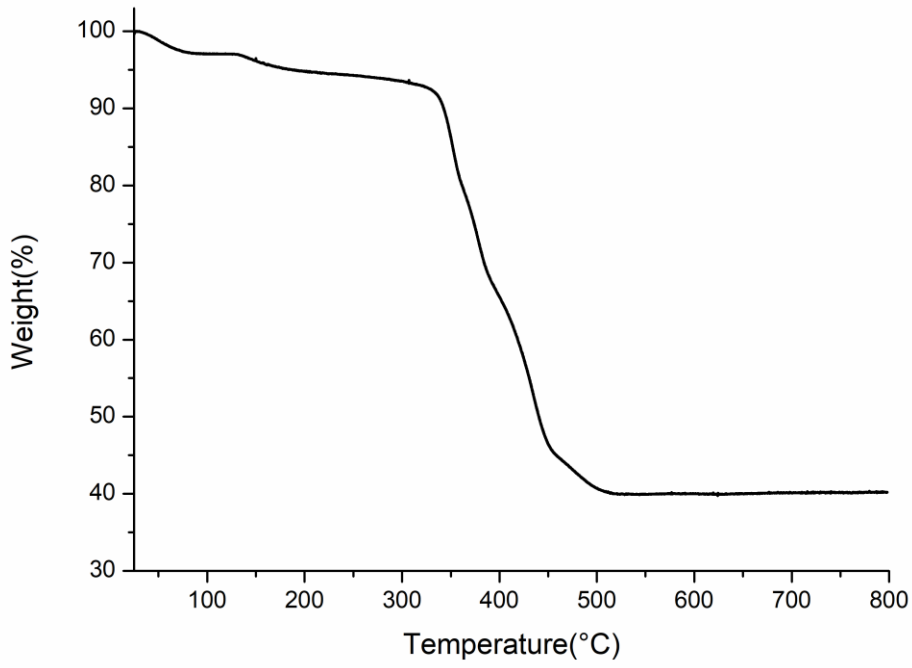

Figure S6. TGA curves of **1**.

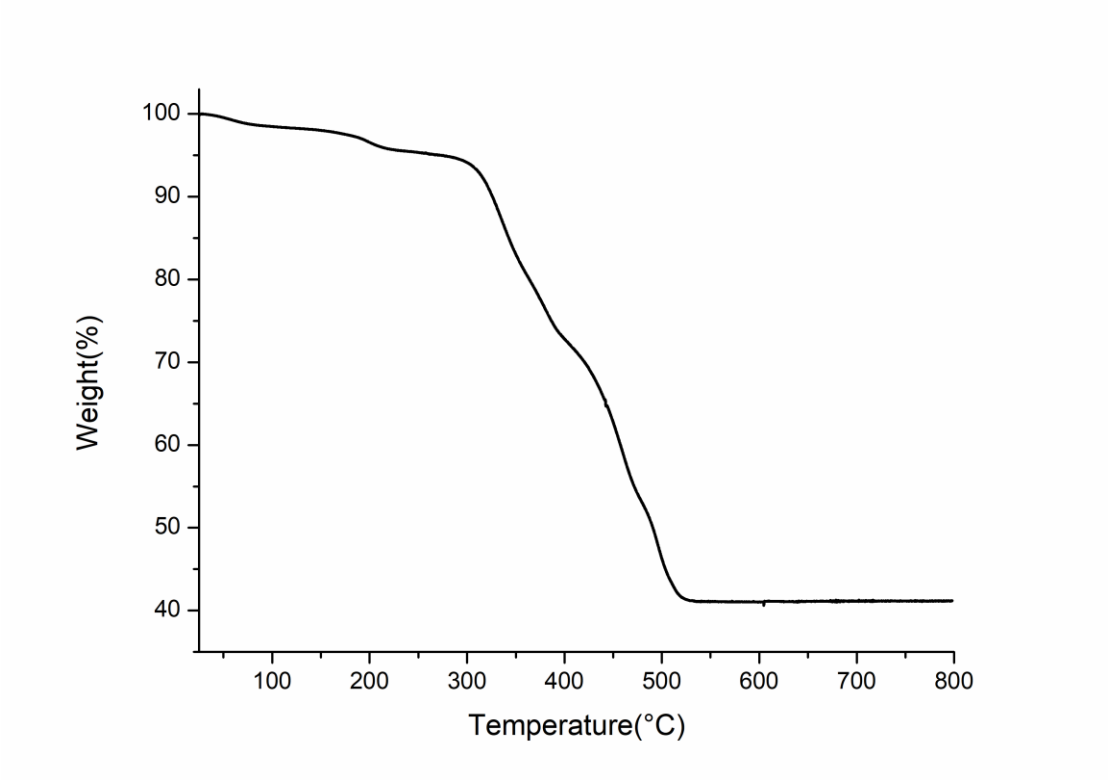

Figure S7. TGA curves of **2**.

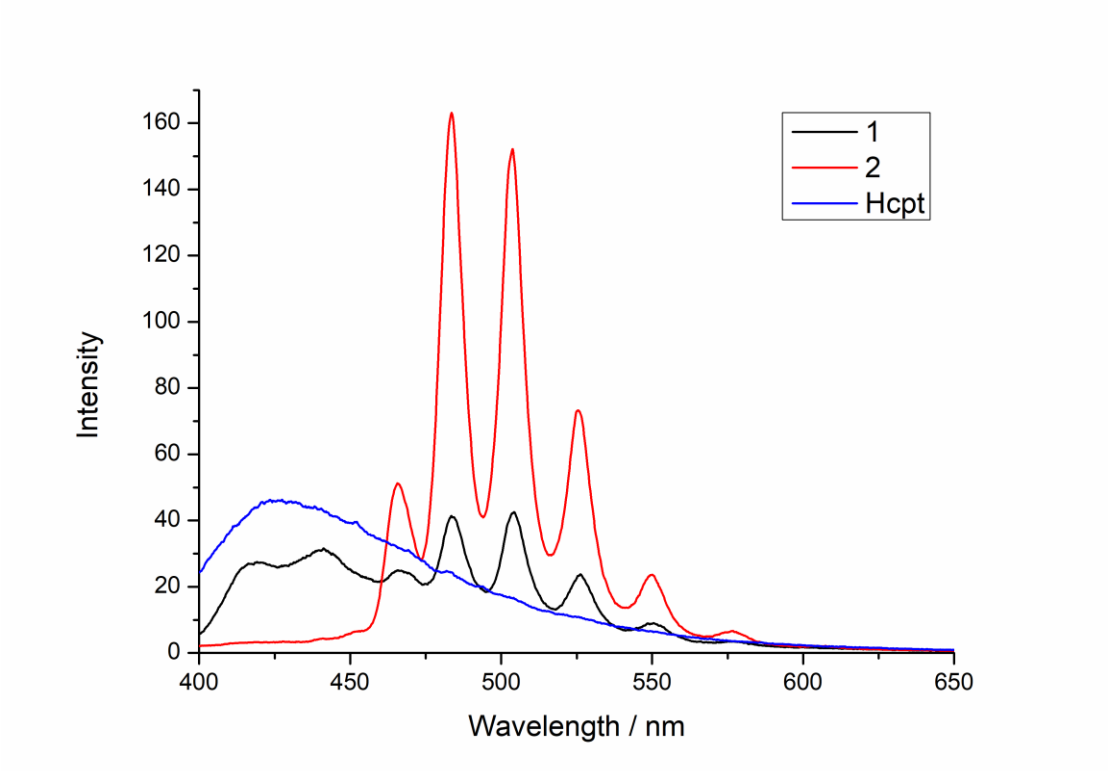

Figure S8. The emission spectra of **1**, **2**, and Hcpt in the solid state at room temperature.