Silver Ion-Mediated Heterometallic Three-Fold Interpenetrating Uranyl-Organic Framework

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Supporting Information

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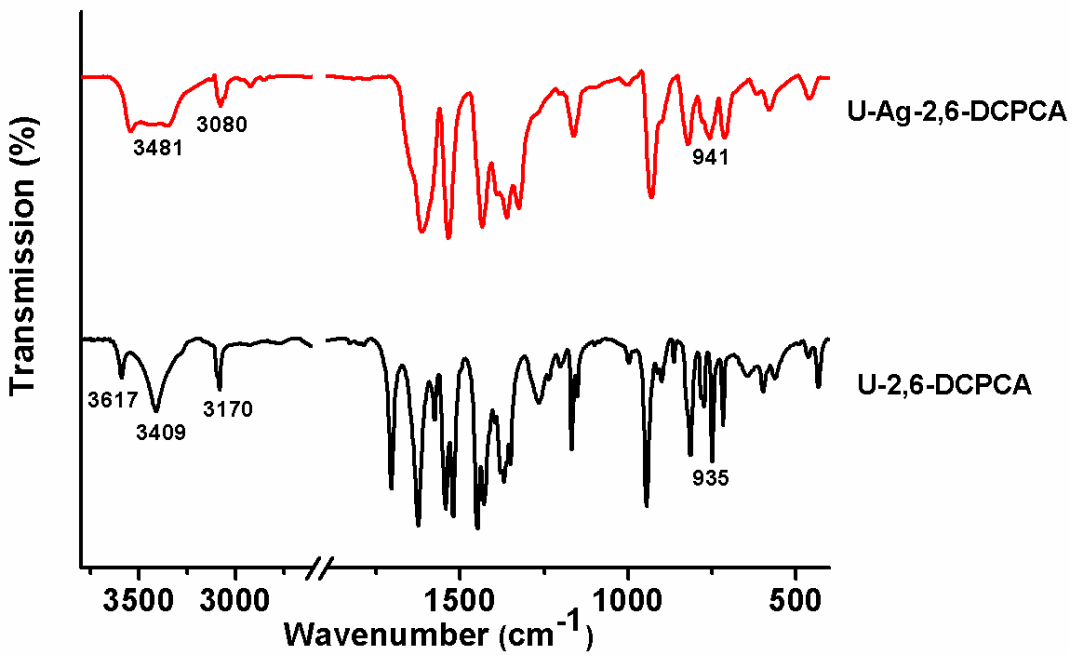

Figure S1. IR spectrum of U-Ag-2,6-DCPCA with that of U-2,6-DCPCA as a compassion.

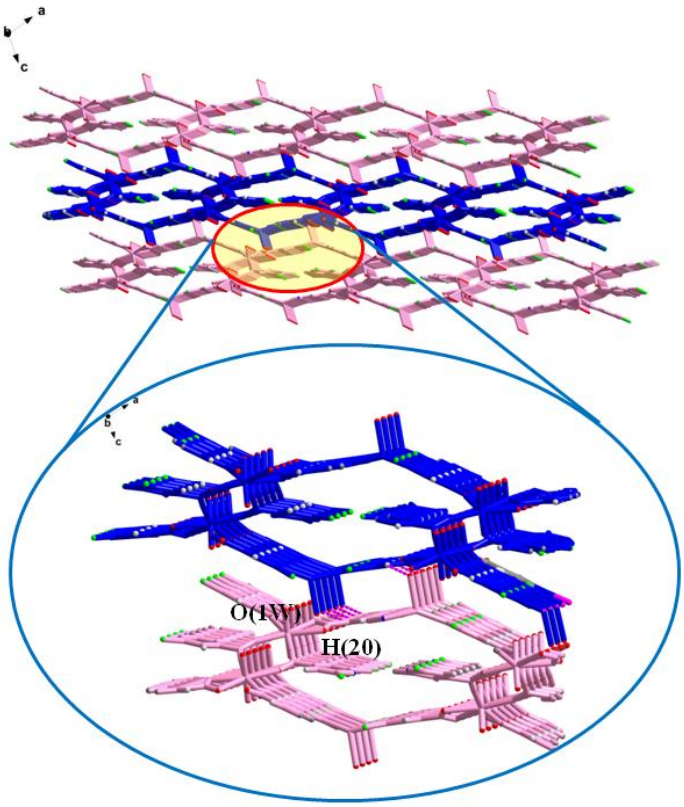

Figure S2. Crystal packing of three-fold interpenetrating network along c axis through hydrogen bonds between different sets of two-dimensional networks via O(1W) and H(20).

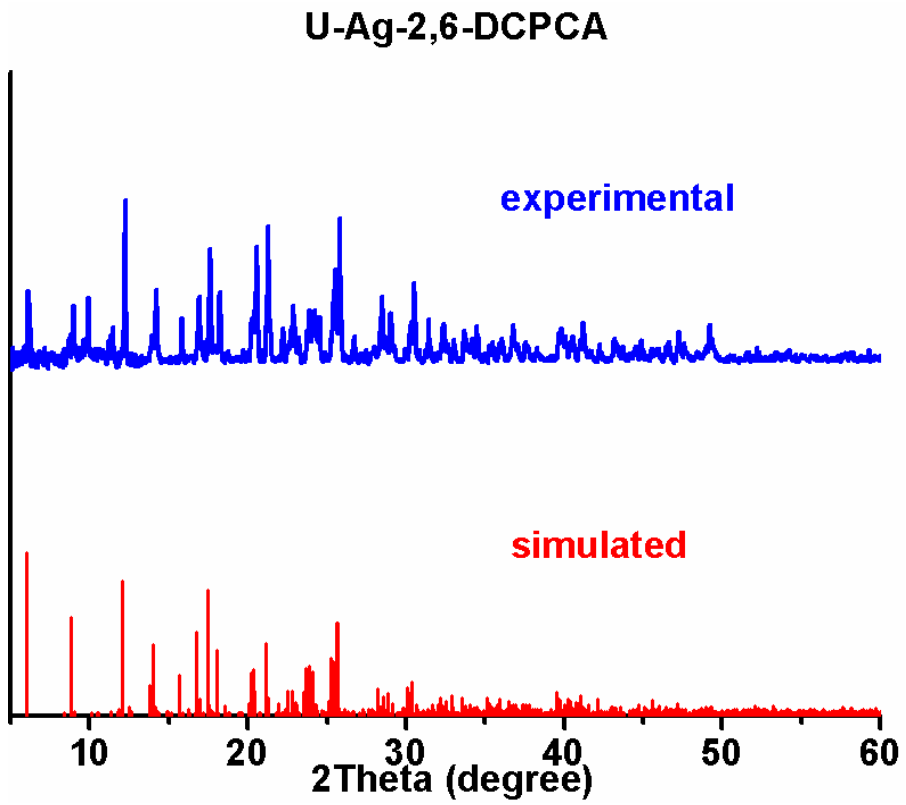

Figure S3. Powder x-ray diffraction of U-Ag-2,6-DCPCA. The experimental spectrum (upper diagram) is in good accordance with the simulated spectra from single crystal data (lower diagram).

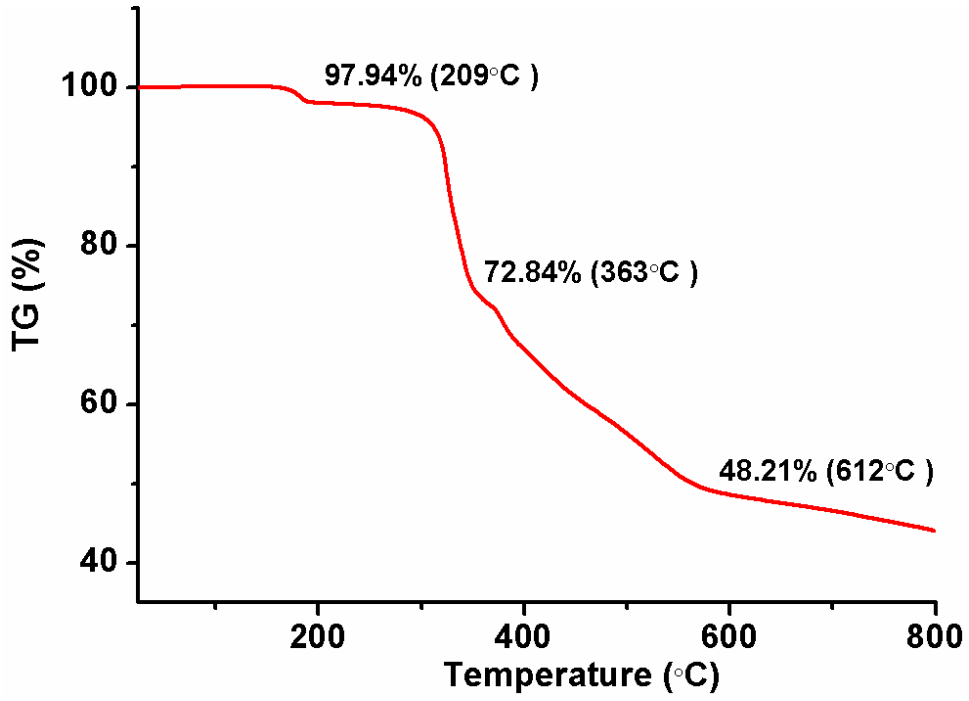

Figure S4. Thermogravimetric result of U-Ag-2,6-DCPCA.

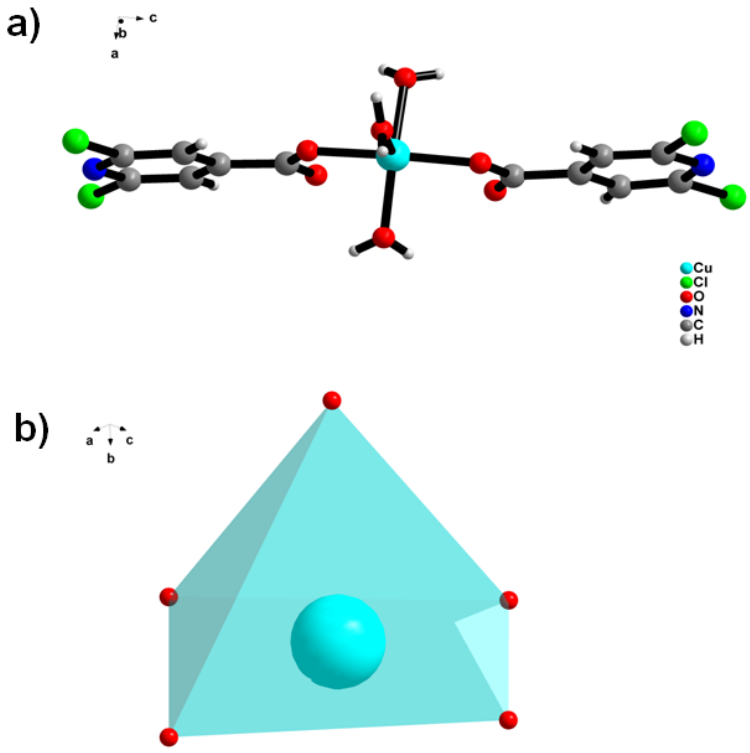

Figure S5. The asymmetric unit of Cu-2,6-DCPCA and the tetragonal pyramid of copper(Cu^{2+}) center.

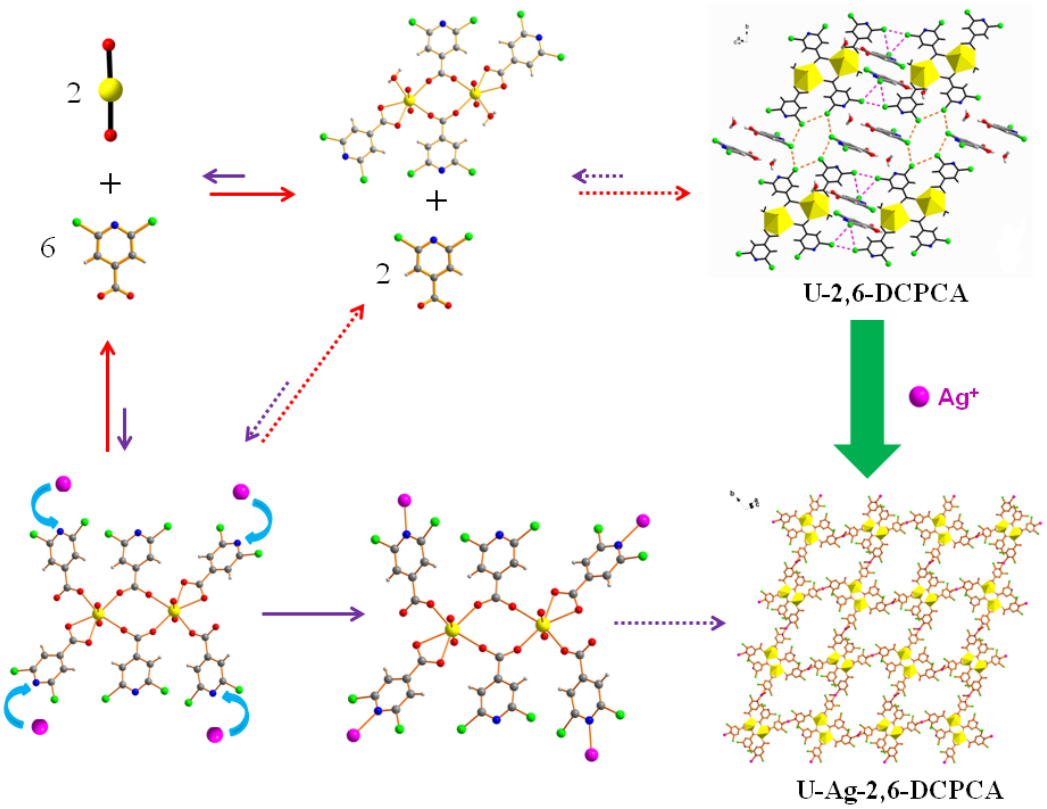

Figure S6. The possible process for the transformation from U-2,6-DCPCA to U-Ag-2,6-DCPCA.

Table S1. Selected uranium-related bond distances (Å) and bond angle (˚) in U-Ag-2,6-DCPCA.

Bond distances /Å			
U(1)-O(1)	1.765(4)	U(2)-O(3)	1.750(4)
U(1)-O(2)	1.759(4)	U(2)-O(4)	1.752(4)
U(1)-O(5)	2.285(4)	U(2)-O(10)	2.336(4)
U(1)-O(6)	2.491(4)	U(2)-O(11)	2.337(4)
U(1)-O(7)	2.518(4)	U(2)-O(12)	2.486(4)
U(1)-O(8)	2.342(4)	U(2)-O(13)	2.521(4)
U(1)-O(9)	2.342(4)	U(2)-O(14)	2.293(4)
Ag1-O(2W)	2.377(6)	Ag2-O(1W)	2.400(4)
Ag1-N(4)	2.292(5)	Ag2-O(1W)	2.286(5)
Ag1-N(3)	2.238(5)	Ag2-O(1W)	2.241(5)
Bond angles /˚			
O(1)-U(1)-O(2)	177.42(19)	O(3)-U(2)-O(4)	177.7(2)
O(1)-U(1)-O(5)	89.05(16)	O(3)-U(2)-O(10)	92.12(17)
O(2)-U(1)-O(5)	93.01(16)	O(4)-U(2)-O(10)	89.33(18)
O(1)-U(1)-O(6)	93.88(17)	O(3)-U(2)-O(11)	87.03(16)
O(2)-U(1)-O(6)	85.19(17)	O(4)-U(2)-O(11)	91.43(16)
O(1)-U(1)-O(7)	84.64(16)	O(3)-U(2)-O(12)	85.41(17)
O(2)-U(1)-O(7)	92.90(17)	O(4)-U(2)-O(12)	94.02(18)
O(1)-U(1)-O(8)	89.79(17)	O(3)-U(2)-O(13)	93.81(17)
O(2)-U(1)-O(8)	92.05(17)	O(4)-U(2)-O(13)	84.08(17)
O(1)-U(1)-O(9)	91.44(16)	O(3)-U(2)-O(14)	93.28(16)
O(2)-U(1)-O(9)	87.10(16)	O(4)-U(2)-O(14)	88.75(16)

Table S2. Crystal data and structure refinement for Cu-2,6-DCPCA.

	Cu-2,6-DCPCA
formula	$C_{12}H_{10}Cl_4N_2O_7Cu$
formula weight	499.56
crystal system	orthorhombic
space group	*P*nab
a, Å	6.9230(14)
b, Å	14.227(3)
c, Å	20.203(4)
α, deg	90
β, deg	90
γ, deg	90
V, Å^3	1989.9(7)
Z	4
T, K	293
Dc, g/cm^3	1.668
μ (Mo K$_\alpha$) (mm^{-1})	1.669
Theta(Min, Max) [Deg]	1.75, 25.12
F(000)	996
R_1, wR_2 [I ≥ 2σ(I)]	0.0357, 0.0969
R_1, wR_2 (all data)	0.0375, 0.0981
Residue Dens. [e/Ang^3]	-0.472, 0.711

Table S3. Selected uranium-related bond distances (Å) and bond angle (˚) in Cu-2,6-DCPCA.

Bond distances /Å			
Cu(1)-O(1)	1.960(2)	Cu(1)-O(1W)	2.139(3)
Cu(1)-O(2W)	1.965(2)		
Bond angles /˚			
O(1)- Cu(1)-O(1W)	94.40(6)	O(1W)- Cu(1)-O(2W)	97.06(7)
O(1)- Cu(1)-O(1)	171.20(1')	O(1)- Cu(1)-O(2W')	88.62(7)
O(1W)- Cu(1)-O(1W')	165.88(1)	O(1)- Cu(1)-O(2W)	90.21(9)