SUPPORTING INFORMATION

Unusual crystal structure and chirality of uridine 5' -monophosphate coordination polymer

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Content

Section 1 IR Spectra

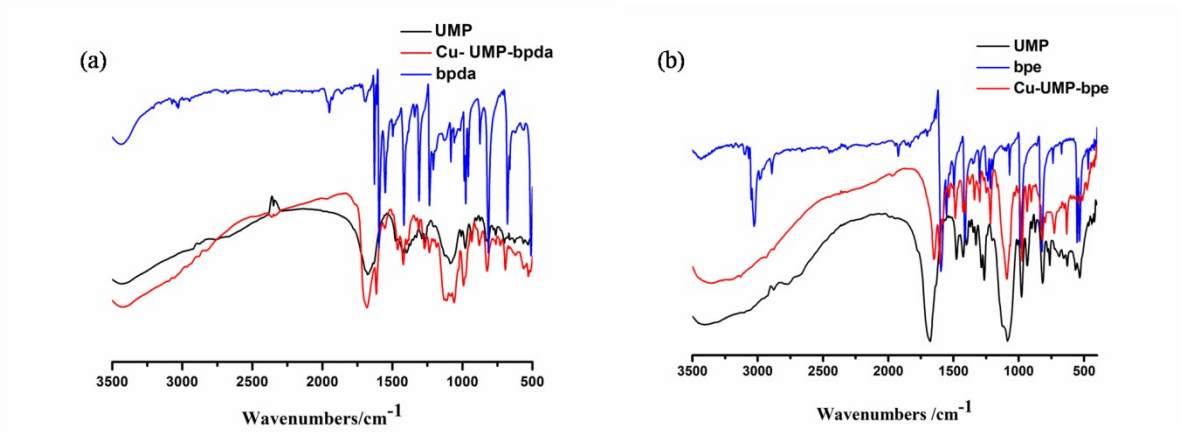

Fig. S1 The infrared spectra of complexes Cu-UMP-bpda/bpe and their ligands.

Section 2 UV-vis Spectra

Table S1. Volume ratio of each compositon in the final solution.

Solution(mL)	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
$V_{Cu\text{-}UMP}$	8	7.5	7	6.5	6	5.5	5	4.5	4	3.5	3	2.5	2	1.5	1	0.5	0
$V_{auxiliary\ ligand}$	0	0.5	1	1.5	2	2.5	3	3.5	4	4.5	5	5.5	6	6.5	7	7.5	8

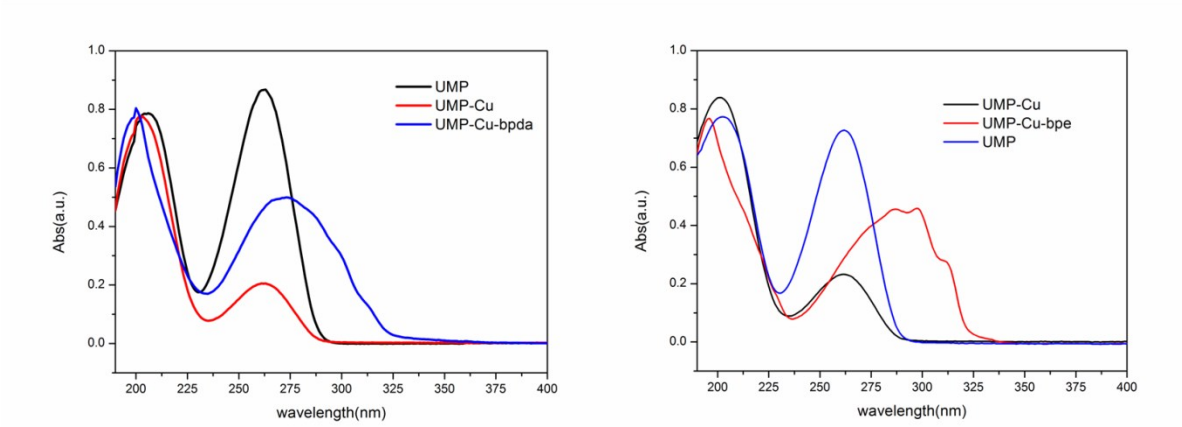

Fig. S2 The UV-vis profile of complexes Cu-UMP-bpda/bpe and their ligands. [UMP] = 1.0×10^{-4} mol/L, [UMP-Cu] = 3.0×10^{-5} mol/L (UMP:Cu = 1:1), [UMP-Cu-bpda] = 3.0×10^{-5} mol/L, [UMP-bpe-Cu] = 3.0×10^{-5} mol/L..

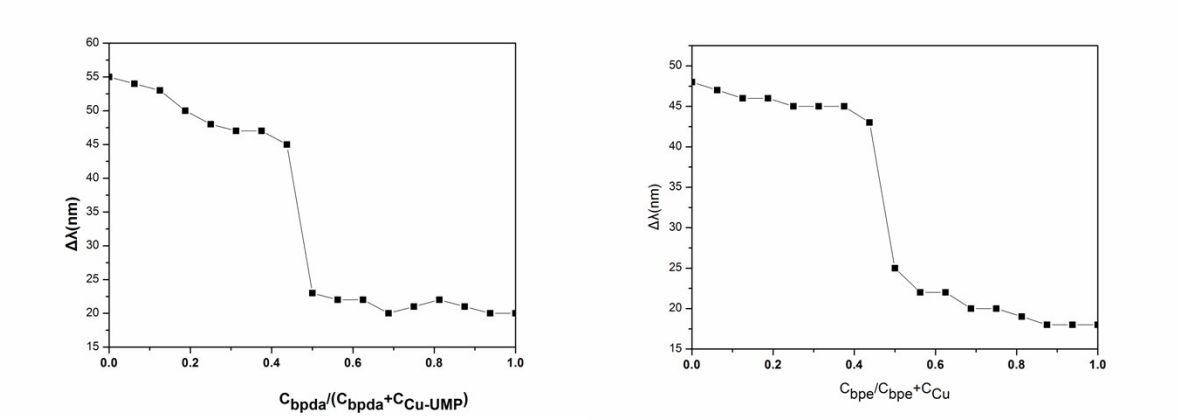

Fig. S3 Plot of the complex formation of Cu-UMP-bpda/bpe, monitored with a UV spectrophotometer.

Section 3 Crystallography Structural graphs

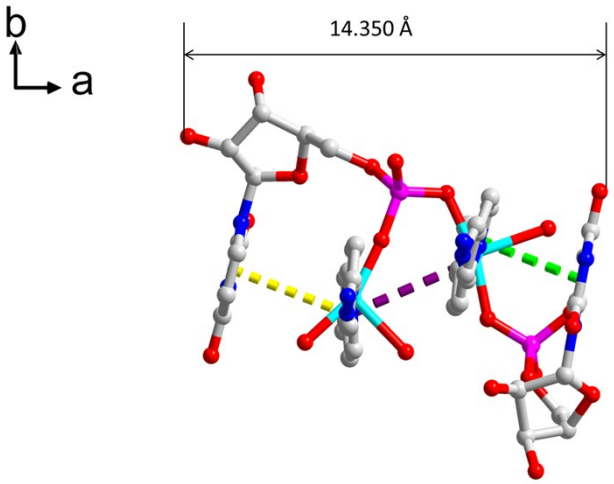

Fig. S4 The belt width of **1**.

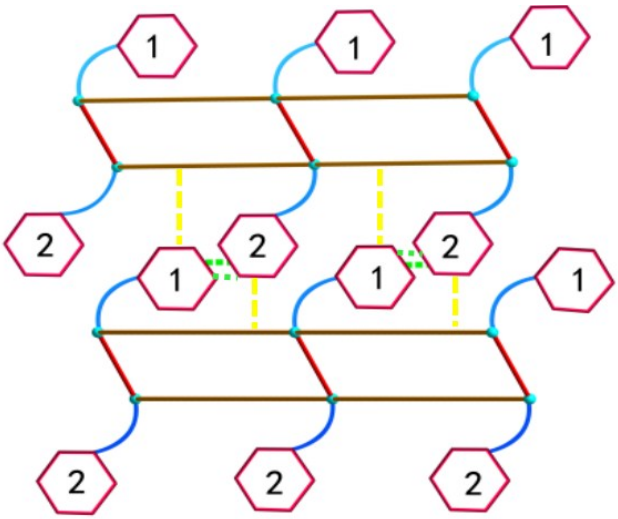

Fig. S5 Cartoon picture used to express the interaction between 1D double bridges visually.

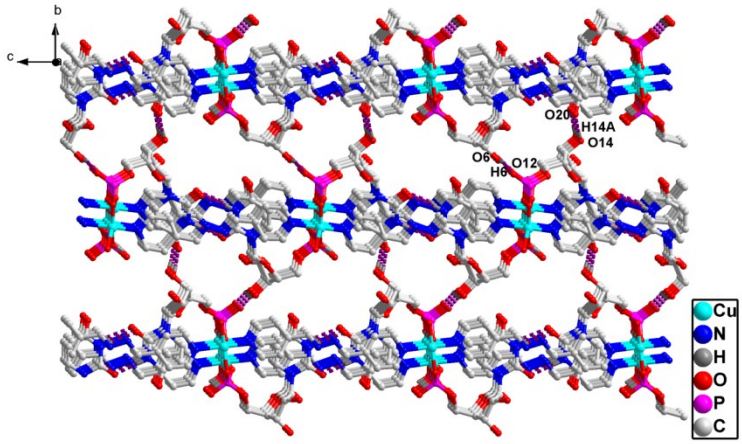

Fig. S6 3D supramolecular framework based on hydrogen bonding viewed down from *a* axis of **1**.

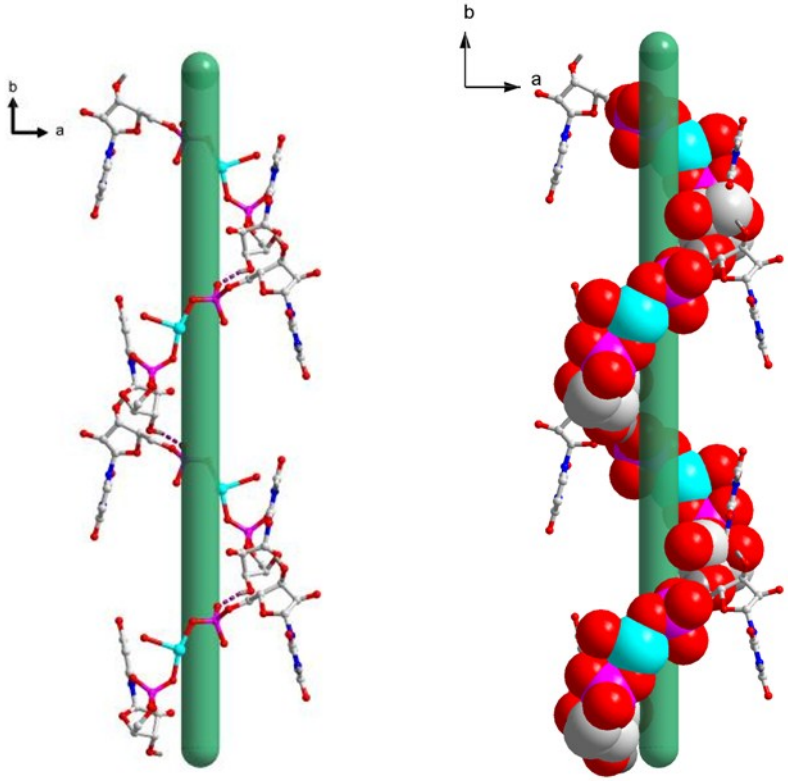

Fig. S7 Helix based on hydrogen bond forming between oxygen of phosphate group and hydroxy group of pentose of **1**.

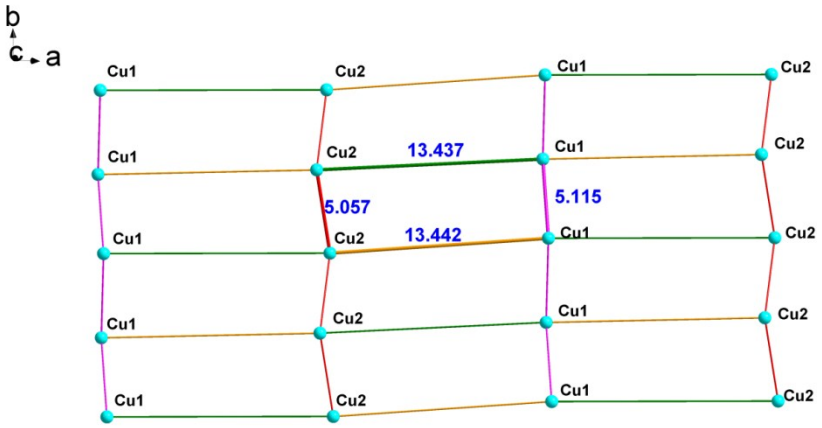

Fig. S8 The Cu···Cu distances in 2D fremwork of complex **2** view down from *c* axis.

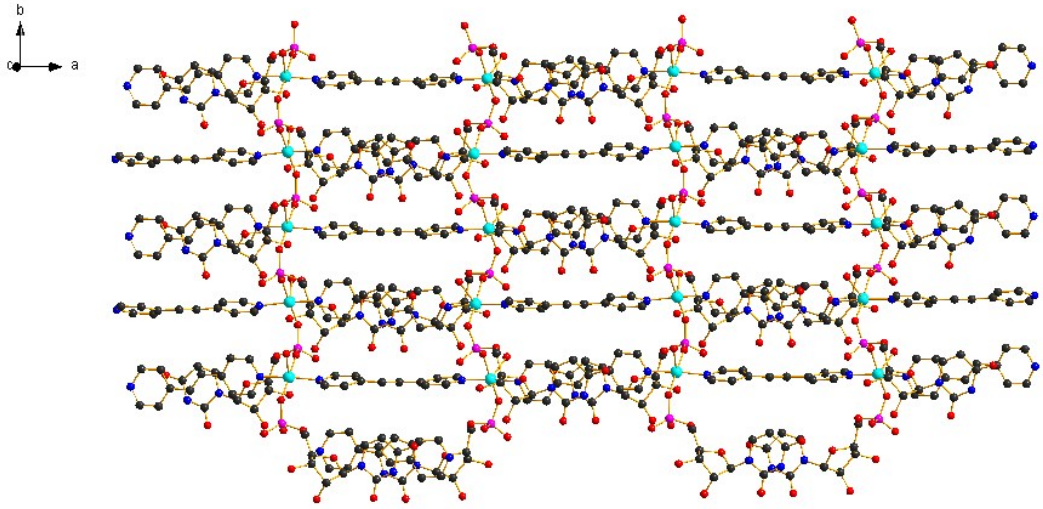

Fig. S9 2D coordination network of complex **2** view down from *c* axis.

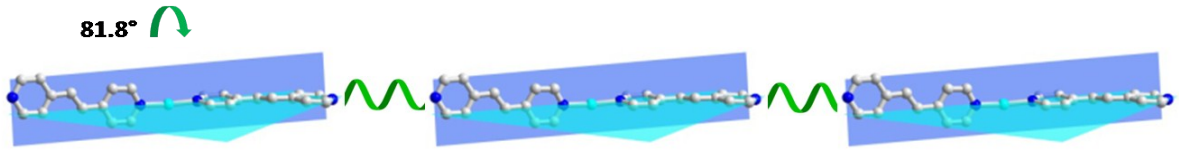

Fig. S10 The dihedral between the adjacent bpe of **2**.

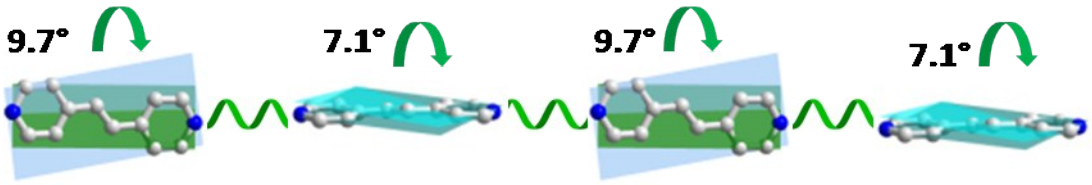

Fig. S11 The dihedral angle of the bpe is 9.7° (*ab* plane) and 7.1° (vector direction) respectively of **2**.

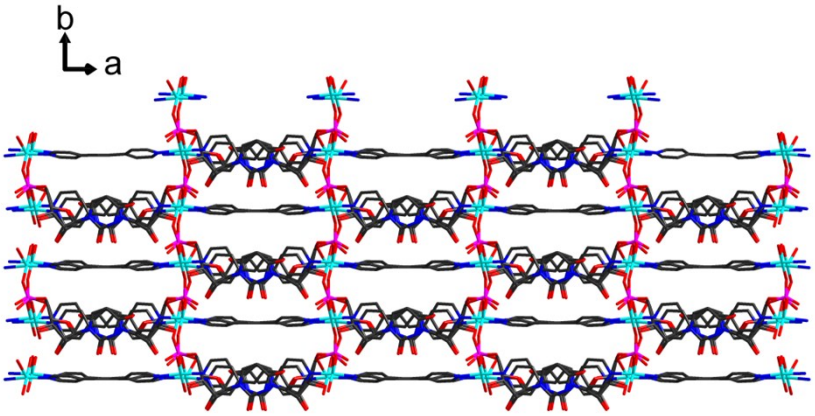

Fig. S12 3D supramolecular architecture of complex **2**.

Section 4 Selected bond distances (Å) and angles (°) of complexes 1–2.

Table S2 Selected bond Distances (Å) and Angles (°) for Complex **1**.

Bond lengths (Å)		Bond angles (°)	
Cu(1)–O(10)	1.880(8)	O(10)–Cu(1)–O(18)	158.4(4)
Cu(1)–O(18)	1.967(9)	O(10)–Cu(1)–N(4)	91.9(4)
Cu(1)–N(4)	2.011(9)	O(18)–Cu(1)–N(4)	89.7(4)
Cu(1)–N(1)#1	2.056(9)	O(10)–Cu(1)–N(1)#1	90.8(4)
Cu(1)–O(19)	2.231(9)	O(18)–Cu(1)–N(1)#1	87.0(4)
Cu(2)–O(1)	1.959(8)	N(4)–Cu(1)–N(1)#1	176.6(4)
Cu(2)–O(11)	1.961(8)	O(10)–Cu(1)–O(19)	109.0(4)
Cu(2)–N(8)	2.036(10)	O(18)–Cu(1)–O(19)	92.6(4)
Cu(2)–N(5)#1	2.051(9)	N(4)–Cu(1)–O(19)	88.8(4)
Cu(2)–O(21)	2.338(9)	N(1)#–Cu(1)–O(19)	92.2(4)
O(10)–P(2)	1.539(9)	O(1)–Cu(2)–O(11)	165.6(3)
O(11)–P(2)	1.519(9)	O(1)–Cu(2)–N(8)	90.2(4)
O(12)–P(2)	1.529(9)	O(11)–Cu(2)–N(8)	90.4(4)
O(13)–P(2)	1.598(9)	O(1)–Cu(2)–N(5)#1	89.8(4)
		O(11)–Cu(2)–N(5)#1	88.5(4)
		N(8)–Cu(2)–N(5)#1	175.3(4)
		O(1)–Cu(2)–O(21)	98.2(3)
		O(11)–Cu(2)–O(21)	96.1(3)
		N(8)–Cu(2)–O(21)	90.7(4)
		N(5)#1–Cu(2)–O(21)	94.0(4)

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

Table S3 H-bonding Distances (Å) and Angles (°) for Complex **1**.

D–H	**d(D–H)**	**d(H···A)**	**∠DHA**	**d(D···A)**	**A**
N10–H10A	0.860	2.023	170.94	2.876	O17 [x+1, y, z+1]
N12–H12	0.860	1.935	168.33	2.782	O8 [x-1, y, z-1]
O6–H6	0.820	1.891	163.24	2.687	O12 [-x+2, y-1/2, -z+2]
O7–H7	0.820	1.995	158.66	2.775	O22 [-x+1, y-1/2, -z+2] O14–
H14A	0.820	1.727	174.96	2.545	O20 [-x+1, y+1/2, -z+1]
O15–H15A	0.820	2.060	175.85	2.879	O28
O18–H18B	0.850	2.069	141.38	2.784	O31
O18–H18C	0.850	1.701	167.63	2.538	O3 [x-1, y, z]
O19–H19C	0.850	1.904	170.57	2.746	O1
O19–H19D	0.850	1.902	170.54	2.744	O26
O21–H21B	0.850	1.965	140.18	2.674	O3
O21–H21C	0.850	1.927	162.47	2.749	O25 [x+1, y, z]
O22–H22C	0.850	1.857	179.75	2.707	O12 [x-1, y, z]
O22–H22D	0.850	2.076	179.25	2.926	O24 [-x+1, y+1/2, -z+1]

O23-H23C	0.850	2.034	173.63	2.881	O9 [x-1, y, z-1]
O23-H23D	0.850	2.006	173.08	2.852	O31 [-x+1, y+1/2, -z+1]
O24-H24C	0.850	2.308	179.35	3.158	N2
O24-H24D	0.850	1.763	177.52	2.613	O28 [-x+1, y-1/2, -z+1]
O25-H25E	0.850	1.965	174.24	2.812	O6 [-x+2, y+1/2, -z+2]
O25-H25F	0.850	2.036	173.64	2.882	O24 [-x+1, y+1/2, -z+1]
O26-H26C	0.850	2.021	174.23	2.868	O22 [-x+1, y-1/2, -z+2]
O26-H26D	0.850	1.993	174.60	2.841	O23 [-x+1, y-1/2, -z+1]
O27-H27C	0.850	2.076	150.65	2.848	O7 [x-1, y, z-1]
O27-H27D	0.850	2.491	152.23	3.267	O8 [x-1, y, z-1]
O27-H27D	0.850	2.345	113.72	2.798	O20
O28-H28C	0.850	1.864	173.41	2.710	O11 [x-1, y, z]
O28-H28D	0.850	1.644	174.83	2.492	O29 [x-1, y, z]
O29-H29C	0.850	1.717	170.18	2.559	O27 [-x+1, y+1/2, -z+1]
O29-H29D	0.850	2.285	169.82	3.125	O30 [-x+1, y+1/2, -z+1]
O30-H30B	0.850	2.442	113.05	2.883	O2 [x-1, y, z]
O31-H31C	0.850	1.874	178.70	2.724	O2 [x-1, y, z]
O31-H31D	0.850	2.065	179.55	2.915	O14 [-x+1, y-1/2, -z+1]

Table S4 Selected bond Distances (Å) and Angles (°) for Complex **2**.

	Bond lengths (Å)		Bond angles (°)
Cu(1)–O(6)	1.955(6)	O(6)–Cu(1)–O(5)	176.9(2)
Cu(1)–O(5)	1.965(5)	O(6)–Cu(1)–N(2)	89.6(2)
Cu(1)–N(2)	2.017(5)	O(5)–Cu(1)–N(2)	88.5(2)
Cu(1)–N(1)	2.046(5)	O(6)–Cu(1)–N(1)	90.8(2)
Cu(1)–O(8)	2.299(6)	O(5)–Cu(1)–N(1)	90.7(2)
Cu(2)–O(1)	1.958(7)	N(2)–Cu(1)–N(1)	171.7(2)
Cu(2)–O(3)	1.980(7)	O(6)–Cu(1)–O(8)	91.2(2)
Cu(2)–N(4)	2.020(6)	O(5)–Cu(1)–O(8)	91.6(2)
Cu(2)–N(3)	2.029(6)	N(2)–Cu(1)–O(8)	101.4 (2)
Cu(2)–O(22)	2.324(13)	N(1)–Cu(1)–O(8)	86.9(2)
P(3)–O(5)	1.503(5)	O(1)–Cu(2)–O(3)	168.2(3)
P(3)–O(10)	1.526(6)	O(1)–Cu(2)–N(4)	89.8(3)
P(3)–O(6)#1	1.531(6)	O(3)–Cu(2)–N(4)	87.6(3)
P(3)–O(9)	1.606(5)	O(1)–Cu(2)–N(3)	90.2(3)
P(4)–O(21)	1.474(8)	O(3)–Cu(2)–N(3)	94.0(3)
P(4)–O(3)#2	1.491(7)	N(4)–Cu(2)–N(3)	171.3(3)
P(4)–O(1)	1.548(7)	O(1)–Cu(2)–O(22)	80.3(4)
P(4)–O(2)	1.600(6)	O(3)–Cu(2)–O(22)	88.9(4)
		N(4)–Cu(2)–O(22)	101.9(4)
		N(3)–Cu(2)–O(22)	86.6(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,y+1/2,-z+2 #2 -x-1/2,y-1/2,-z+1 #3 x+1,y,z+ #4 x-1,y,z-1 #5 -x-1/2,y+1/2,-z+1 #6 -x+1/2,y-1/2,-z+2

Table S5 H-bonding Distances (Å) and Angles (°) for Complex **2**.

D–H	d(D–H)	d(H···A)	∠DHA	d(D···A)	A
O8-H8A	0.850	1.927	157.99	2.734	O25 [-x+1/2, y+1/2, -z+2]
O8-H8B	0.820	2.525	152.27	3.274	O16 [x+1/2, y+1/2, z+1]
O12-H12A	0.840	1.929	137.04	2.607	O24
O16-H16A	0.840	1.871	168.04	2.698	O6 [x-1/2, y-1/2, z-1]
O17-H17A	0.851	2.044	166.40	2.878	O10 [-x, y-1, -z+1]

Section 5 PXRD Patterns

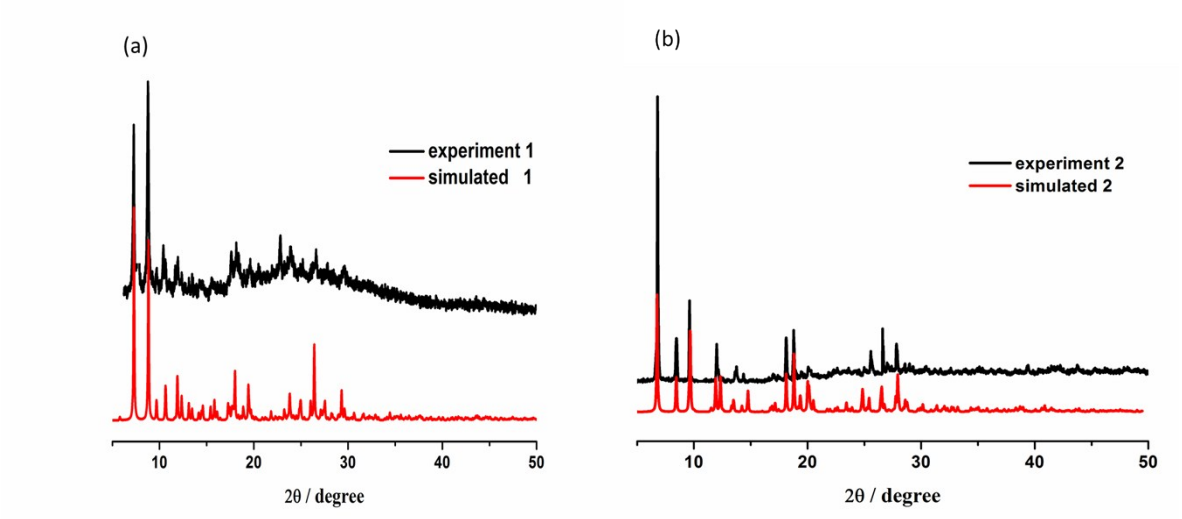

Fig. S13 The experimental PXRD.patterns of Cu-UMP-bpda/bpe (a) (b) is agreement well with its simulated ones, which indicates the phase purity of Cu-UMP-bpda/bpe.

Section 6 TGA Curve

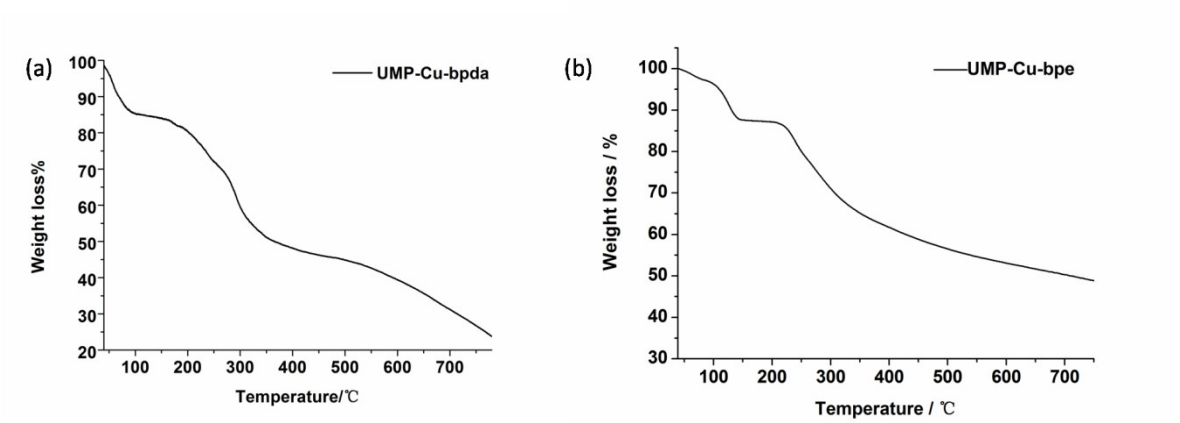

Fig. S14 TGA curve for complexes Cu-UMP-bpda/bpe. (a) The first weight loss due to the removal of in the temperature range 40–100°C is assigned to the loss of ten guest water solvates and three coordinated water molecules (exp. 15.9%, cal. 16.4%), the second weight loss at 200°C corresponding to the decomposition of its backbone. (b) The first weight loss in the temperature range 40–130°C due to the removal of seven guest water solvates and two coordinated water molecules (exp. 12.4%, cal. 12.5%), the second weight loss at 220°C corresponding to the decomposition of its backbone.