Supplementary Information

Controllable synthesis of two Adenosine 5' - monophosphate nucleotide coordination polymers by pH regulation: crystal structure and chirality

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Content

1. Section 1 IR Spectra

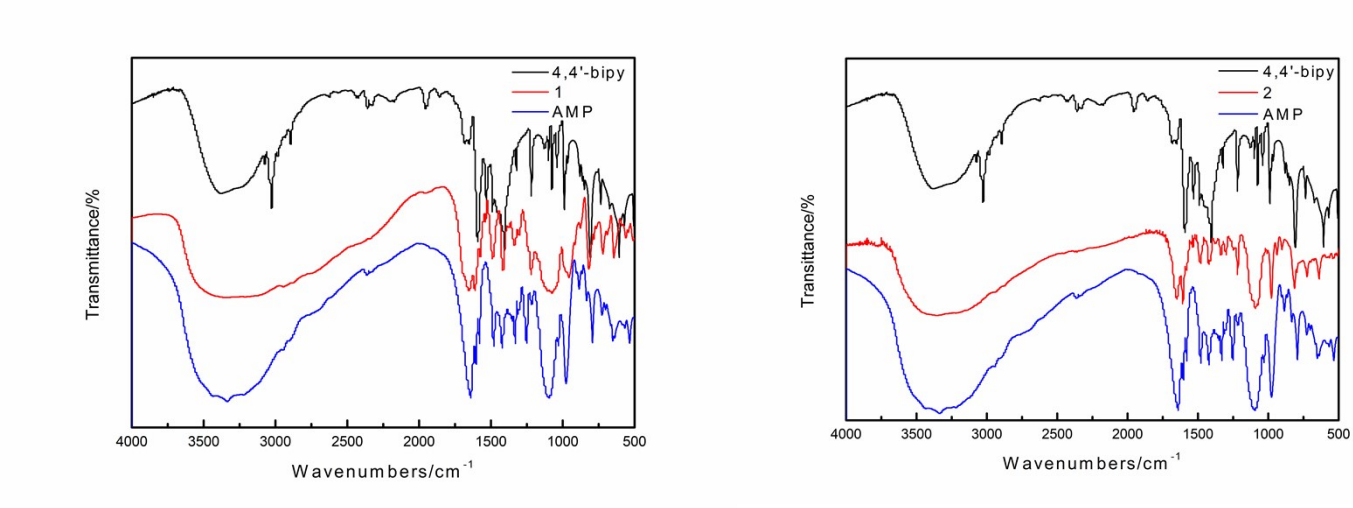

Fig. S1 The infrared spectra of complexes 1,2 and their ligands.

2. Section 2 UV-vis Spectra

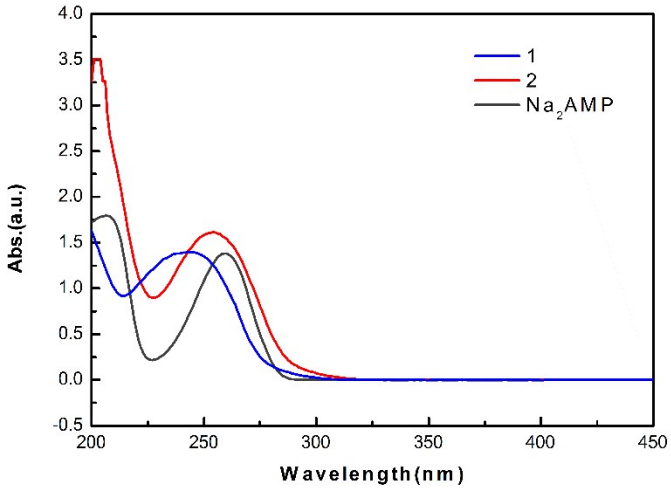

Fig. S2 The UV-vis profile of complexes 1(blue line), 2 (red line)and Na_2AMP ligands(black line). $[Na_2AMP]=[1]=[2] =5.0\times10^{-5}$ mol L^{-1}.

3. Crystallography Structural Graphs

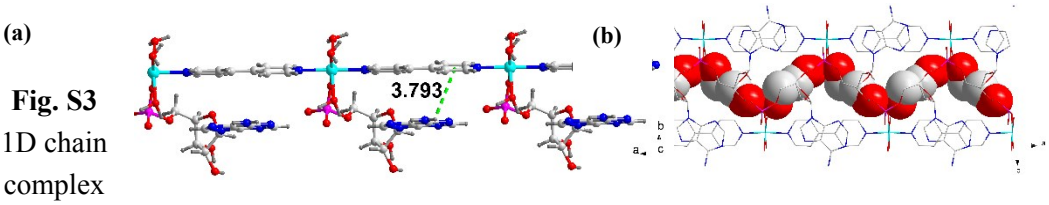

Fig. S3 1D chain complex (a) of **1** viewed down from *c* axis. (b) Chiral helical canister of 1 viewed down from *b* axis.

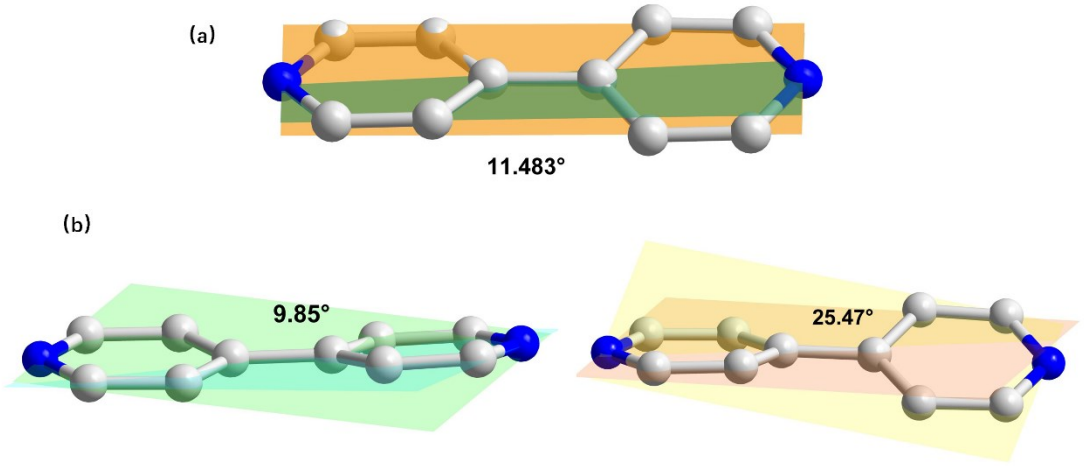

Fig. S4 Dihedral Angle of 4, 4 '-bipy in 1 (a) and 2 (b).

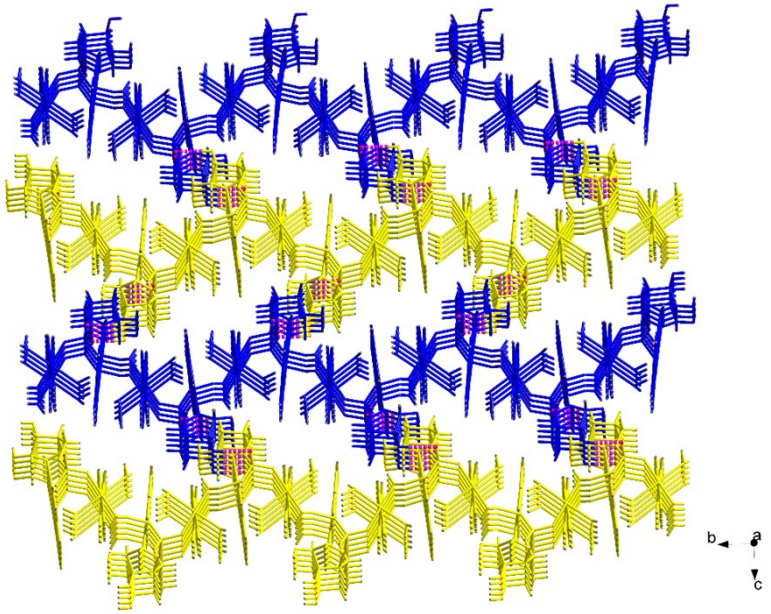

Fig. S5 3D supramolecular framework of complexes **1** based on H-bonding (O10–H19…O11, 1.948Å, 2.768Å, 178.67°).

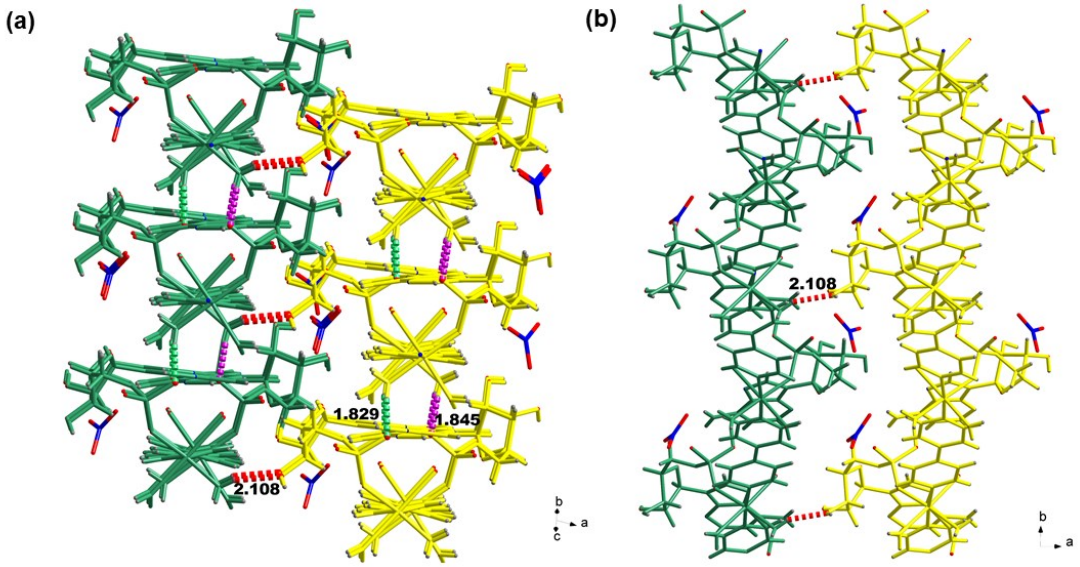

Fig. S6 3D supramolecular framework of complexes 2 based on H-bonding (O16···H16B-O19:2.109Å, 2.889Å, 154.32°).

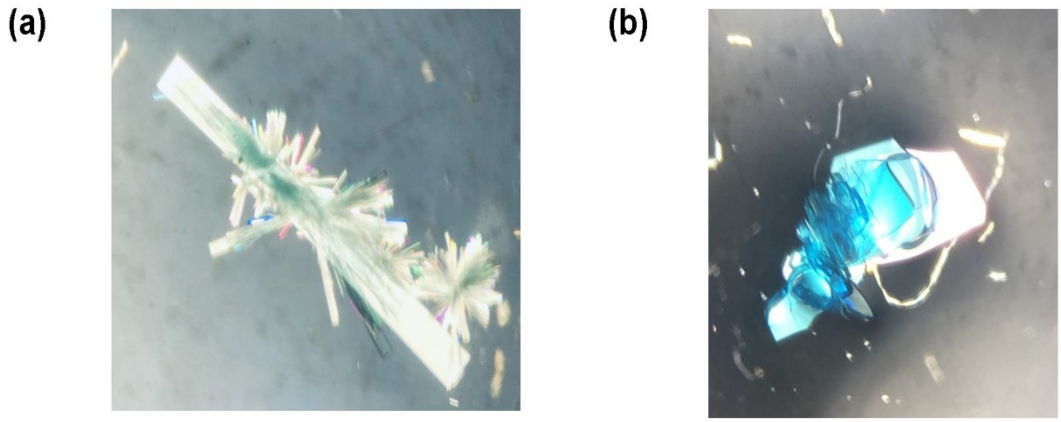

Fig. S7 Pictures of **1**(a, blue-green rod-shaped crystal) and **2** crystals(b, blue bulk crystal).

4. Selected bond distances (Å) and angles (°) for complexes 1 and 2

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Cu1-O4	2.348(7)	Cu1-O8	1.982(6)
Cu1-O9	1.965(4)	Cu1-O13	2.344(7)
Cu1-N5	2.068(6)	Cu1-N1_b	2.070(6)
O4-Cu1-O8	86.3(2)	O4-Cu1-O9	94.2(2)
O4-Cu1-O13	174.8(3)	O4-Cu1-N5	91.1(3)
O4-Cu1-N1_b	87.0(3)	O8-Cu1-O9	176.9(2)
O8-Cu1-O13	92.9(2)	O8-Cu1-N5	86.5(2)
O8-Cu1-N1_b	91.5(2)	O9-Cu1-O13	86.8(2)
O9-Cu1-N5	90.4(2)	O9-Cu1-N1_b	91.6(2)
O13-Cu1-N5	94.0(2)	O13-Cu1-N1_b	87.9(2)
N5-Cu1-N1_b	177.3(2)		

Table S2 Selected H-bonding distances (Å) and angles (°) for complex **1**.

D-H	d(D-H)	d(D···H)	∠DHA	d(D···A)	A	Symmetry
O4-H16	1.048	1.867	148.60	2.815	O14	
O8-H18	0.892	1.776	158.45	2.626	O6	
O8-H17	0.893	1.831	150.18	2.644	O7	[-x+1, y-1/2, -z+1/2]
O10-H19	0.820	1.948	178.67	2.768	O11	[x+1/2, -y+3/2, -z+1]
N7-H20	0.860	2.122	166.12	2.964	O15	[x+1, y, z]
N7-H21	0.860	2.618	158.93	3.435	O5	
O13-H23	0.903	1.967	150.37	2.788	O14	[-x+1, y-1/2, -z+1/2]

TableS3. Selected bond distances(Å) and angles(°) for **2**

Cu(1)–O(1)	1.945(2)	Cu(1)–O(6)	2.013(2)
Cu(1)–N(1)	2.020(3)	Cu(1)–N(2)	2.023(3)
Cu(1)–O(7)	2.336(3)	Cu(2)–O(11)	1.950(2)
Cu(2)–O(15)	2.371(3)	Cu(2)–N(4)	2.009(3)
Cu(2)–O(16)	2.021(2)	Cu(2)–N(3)	2.029(3)
O(1)–Cu(1)–O(6)	177.59(10)	O(1)–Cu(1)–N(1)	89.06(10)
O(6)–Cu(1)–N(1)	90.63(10)	O(1)–Cu(1)–N(2)	93.66(11)
O(6)–Cu(1)–N(2)	86.85(11)	N(1)–Cu(1)–N(2)	174.52(12)
O(1)–Cu(1)–O(7)	91.53(10)	O(6)–Cu(1)–O(7)	86.08(10)
N(1)–Cu(1)–O(7)	89.31(11)	N(2)–Cu(1)–O(7)	95.36(10)
O(11)–Cu(2)–N(4)	90.77(11)	O(11)–Cu(2)–O(16)	174.64(10)
N(4)–Cu(2)–O(16)	87.58(11)	O(11)–Cu(2)–N(3)	91.80(11)
N(4)–Cu(2)–N(3)	175.27(13)	O(16)–Cu(2)–N(3)	90.21(11)
O(11)–Cu(2)–O(15)	82.36(10)	N(4)–Cu(2)–O(15)	93.13(11)
O(16)–Cu(2)–O(15)	92.63(10)	N(3)–Cu(2)–O(15)	91.15(11)

Table S4 Selected H-bonding distances (Å) and angles (°) for complex **2**.

D-H	d(D-H)	d(D···H)	∠DHA	d(D···A)	A	Symmetry
N9-H9B	0.860	1.955	174.17	2.812	O13	
N9-H9C	0.860	2.150	154.53	2.950	O21	[x-1, y, z]
N12-H12A	0.860	2.054	158.50	2.872	O2	[x, y-1, z-1]
N12-H12B	0.860	2.219	154.56	3.018	O34	[x, y, z-1]
N7-H77	1.074	1.622	157.50	157.50	O12	
O6-H6D	0.850	1.818	171.68	2.662	O12	[x, y, z+1]
O6-H6	0.820	1.958	169.25	2.768	O30	[x, y, z+1]
O7-H7	0.820	1.963	169.28	2.773	O28	[x, y, z+1]
O9-H9	0.820	1.881	169.37	2.691	O29	[x+1, y, z]
O10-H10	0.820	2.034	152.36	2.786	O23	
O15-H15E	0.850	2.629	164.24	3.455	O25	[x-1, y-1, z+1]
O15-H15D	0.850	2.014	156.96	2.816	O27	[x, y-1, z]
O16-H16	0.820	1.878	170.58	2.690	O4	[x, y-1, z]
O19-H19	0.820	1.908	163.25	2.704	O33	[x-1, y-1, z]

O7-H71	0.841	2.055	165.14	2.875	O32	[x, y, z+1]
O16-H161	0.897	2.009	169.21	2.895	O19	[x+1, y, z]
O20-H20	0.820	2.268	156.47	3.037	O24	[x-1, y-1, z]

5. X-ray powder diffraction of complexes **1** and **2**

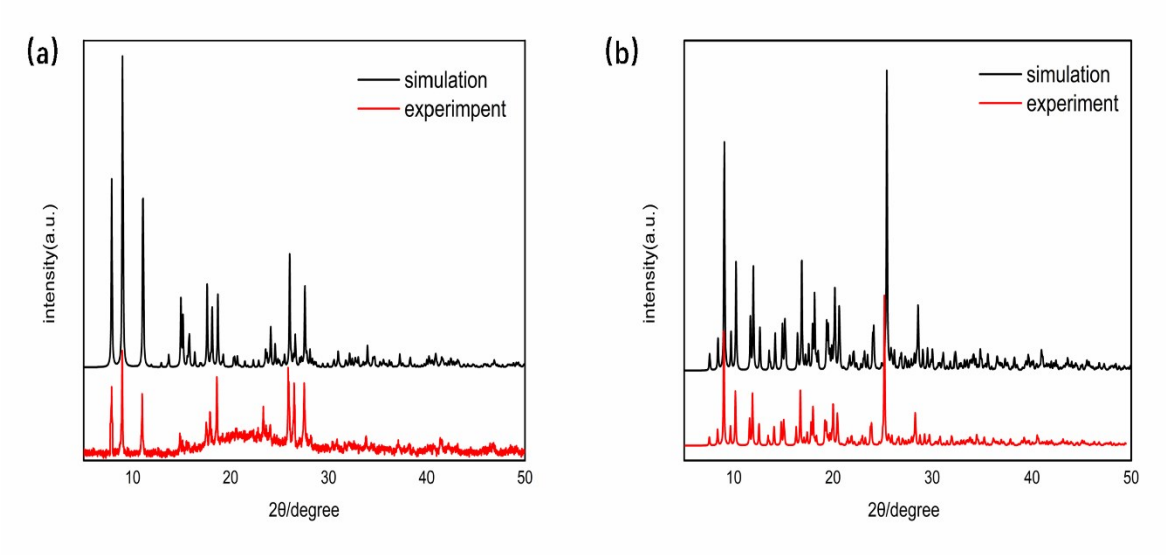

Fig. S8 PXRD patterns show the comparison between the experimental value and calculated ones for complexes **1**(a) and **2**(b)**.**

Under the same conditions, Cu^{2+} were changed into Co^{2+}, and the obtained powder was determined by PXRD.

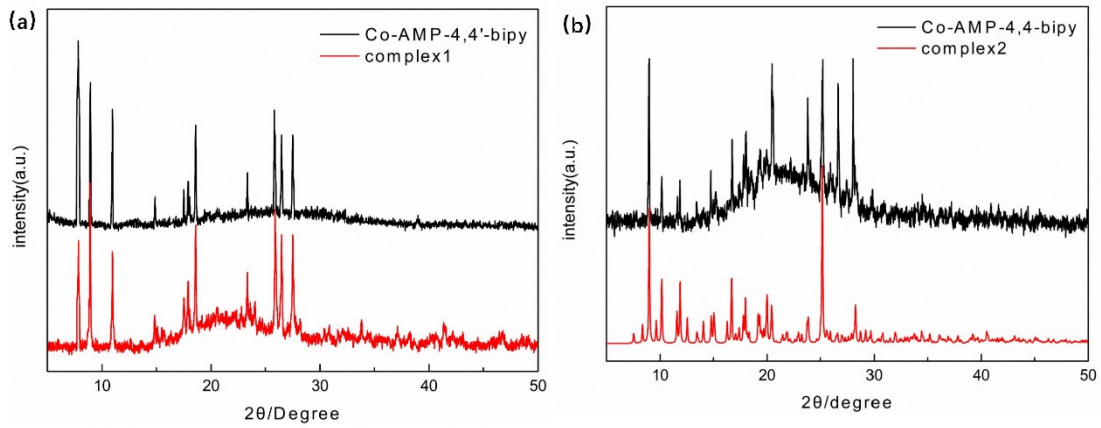

Fig. S9. Comparison of PXRD patterns between Co-AMP-4,4'-bipy and **1** as well as Co-AMP-4,4'-bipy and **2**. It is clearly that complexes of different kinds of metal ions adopt the same structure at similar acidity conditions.

We selected different pHs for experiments. The peak in the PXRD spectrum was basically the same as complex **1** in the pH range of 6.37-5.30. The peak in the PXRD spectrum was basically the same

as complex **2** when the pH value is less than 5.30.

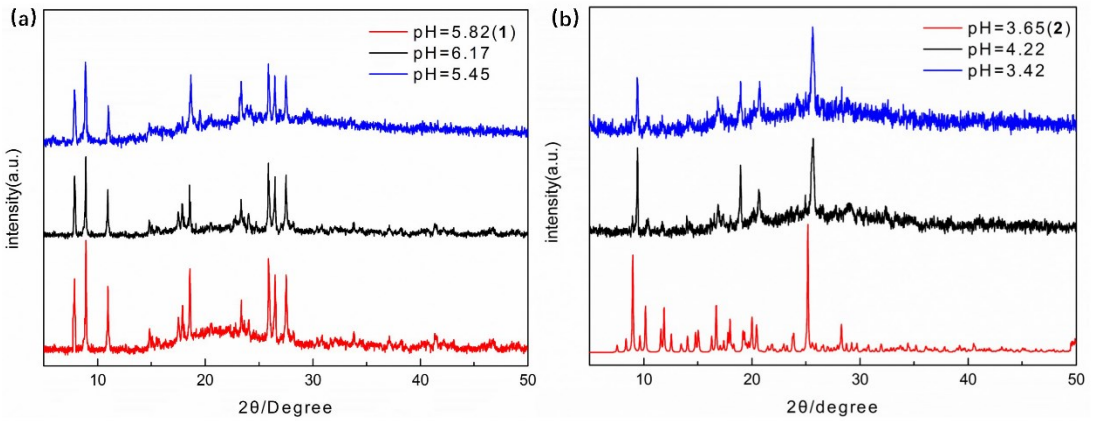

Fig. S10. The power X-ray diffraction pattern of complexes at different pHs. (5.82 and 3.65 correspond to complexes 1 and 2, respectively.)

6. TGA Curve

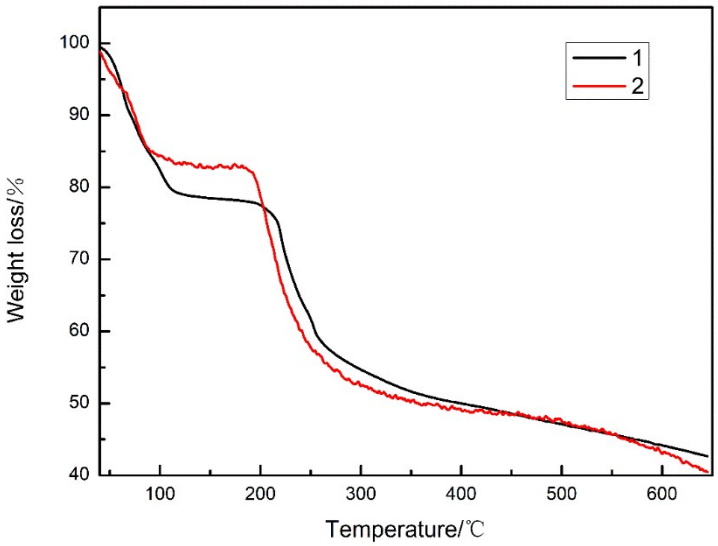

Fig. S11 TGA curve for complexes **1** and **2**. The first weight loss stage of complex **1** occurred from 30.4 ℃ to 130.6 ℃, and the mass loss was 21.20%. The loss of 5 solvent water molecules and 3 coordination water molecules in the complex (theoretical value 20.57%) occurred. When the temperature increased to about 201.1 ℃, the skeleton of complex 1 collapsed(black line). The first seeding stage of complex **2** occurred from 30.9°C to 115.0°C, and the mass loss was 16.73%, corresponding to the loss of 11 solvent water molecules and 4 coordinated water molecules in the complex (theoretical value 17.5%). When the temperature rises to about 190.2℃, the framework of complex **2** collapses(red line).