Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2013

Synthesis and Structural Characterization of a Single-Crystal to Single-Crystal Transformable Coordination Polymer

Yuyang Tian[a], Phoebe K. Allan[a], Catherine L. Renouf[a], Xiang He[b], and Russell E. Morris*[a]

Supporting Information

Elemental Analysis of CHNS

The elemental analysis on C, H, N and S of the products was taken place on a Carlo Erba CHNS analyser. The weight contents of C, H, N and S are 35.94%, 2.51%, 3.65% and 7.05%. The calculated values are 34.49%, 2.43%, 3.10% and 7.08%.

Thermal Stability

The TGA curve of compound 1 was shown in Fig S1. An obvious weight loss of 7.42% ranging from 473K to 513K in air atmosphere can be referred to the removal of the coordinated molecules (calculated weight loss from the complete removal of water is 7.96%).

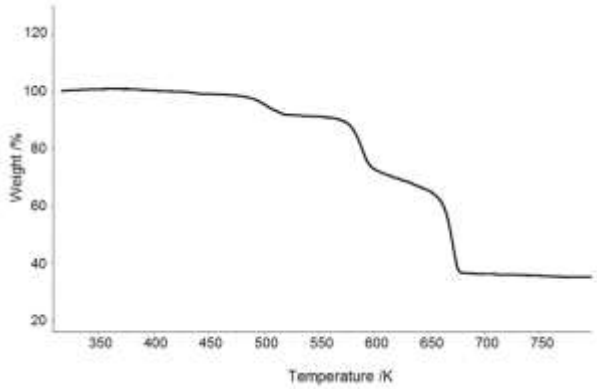

Fig. S1, TGA curve for hydrated sample of compound **1** in air atmosphere at the heating rate of 10Kmin^{-1}.

Compound **1** was put in a tube furnace, heated under air at a 10Kmin^{-1} rate. After calcined at 520K, 540K, 580K and 600K for 10 min respectively, the residuals were recovered to room temperature. Powder XRD was carried on these residuals. The patterns are shown in Fig S2.

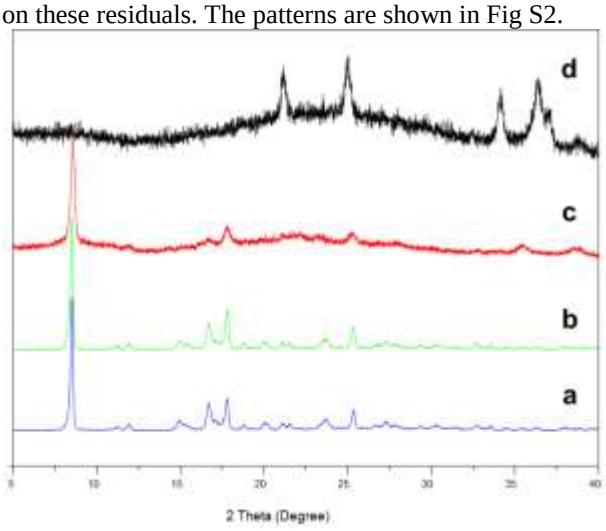

Fig. S2, PXRD pattern of the samples which were calcined at (a) 520K, (b) 540K, (c) 580K and (d) 600K, respectively.

This journal is © The Royal Society of Chemistry 2013

Coordination geometry of Cu-BPy-Cu chain

The coordination geometry of Cu2 in compound **1** is shown in Fig. S3a. It is 6-coordinated by two STP molecules and two Bpy molecules in an inverse way. The changes of Cu2 after dehydration are shown in fig. S3b. The coordination geometry of copper atoms remains 6-coordinated but the Cu-Bpy-Cu chain has a torsion angle of $19.131(821)^0$.

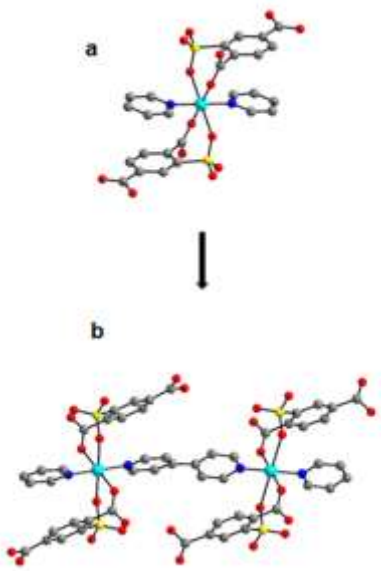

Fig. S3. Coordination environment of Cu2 atoms in hydrated structure (a) and the changes after dehydration (b). (Cu: turquoise, O: red, S: yellow, C: grey, N: blue. H is not shown for clarity.)

Crystallographic data

The crystal data and structure refinements of compound **1** and compound **2** are shown in table S1.

Table S1. Crystal data and structure refinements of compounds **1** and compound **2**

Compound	**1**	**2**
Formula	$C_{26}H_{22}Cu_3N_2O_{18}S_2$	$C_{26}H_{14.5}Cu_3N_2O_{14.25}S_2$
Formula weight	905.20	837.64
Crystal system	Monoclinic	Monoclinic
Space group	P21/c	P21/c
a (Å)	11.017(5)	10.075(5)
b (Å)	11.814(5)	12.806(5)
c (Å)	12.135(5)	19.502(5)
α (º)	90.000(5)	90.000(5)
β (º)	109.701(5)	95.342(5)
γ (º)	90.000(5)	90.000(5)
V ($Å^3$)	1487.0(11)	2505.2(17)

This journal is © The Royal Society of Chemistry 2013

Z	2	4
D_c (g/cm^{-3})	2.022	2.221
F(000)	910	1670
μ (mm^{-1})	2.890	3.411
ϑ for data collection (^{o})	2.85 to 34.65	2.96 to 22.79
Reflections collected	21375	23264
Unique reflections	4736	2610
R_{int}	0.0578	0.0959
Data/restraints/parameters	4736/ 6/ 244	2610 / 0 / 412
Goodness-of-fit on F^2	1.023	1.045
R_1, wR_2 [I >2σ(I)]	0.0327, 0.0904	0.1038, 0.2118
R_1, wR_2 (all data)	0.0378, 0.0938	0.0713, 0.1854

$R_1 = \sum(|F_o| - |F_c|) / \sum|F_o|$, $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$.

Table S2. Selected Bond lengths [Å] for mor20.

Cu(1)-O(3)	1.9321(17)
Cu(1)-O(1W)	1.9757(16)
Cu(1)-O(2W)	1.9909(16)
Cu(1)-O(5)#1	1.9913(16)
Cu(1)-O(9)#2	2.2895(16)
Cu(2)-N(1)#3	1.9744(18)
Cu(2)-N(1)	1.9744(18)
Cu(2)-O(6)	2.0435(16)
Cu(2)-O(6)#3	2.0435(16)
Cu(2)-O(7)	2.2887(17)
Cu(2)-O(7)#3	2.2887(17)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,-y+3/2,z-1/2 #2 -x+2,-y+2,-z+1 #3 -x+3,-y+2,-z+2

#4 x+1,-y+3/2,z+1/2 #5 -x+2,-y+2,-z+2

This journal is © The Royal Society of Chemistry 2013

Table S3. Selected Bond lengths [Å] for mor21.

Cu(1)-O(13)	1.825(8)
Cu(1)-O(11)#1	1.907(10)
Cu(1)-O(12)#1	1.948(9)
Cu(1)-O(1)	1.960(9)
Cu(1)-C(15)#1	2.253(15)
Cu(1)-S(1)	2.769(4)
Cu(2)-O(5)#2	1.856(9)
Cu(2)-O(7)#3	1.869(12)
Cu(2)-O(10)	1.975(10)
Cu(2)-O(6)#3	2.121(14)
Cu(2)-O(9)#4	2.193(10)
Cu(2)-C(8)#3	2.29(2)
Cu(3)-N(2)#5	1.889(12)
Cu(3)-N(2)	1.889(12)
Cu(3)-O(14)	2.027(9)
Cu(3)-O(14)#5	2.027(9)
Cu(3)-O(8)	2.334(10)
Cu(3)-O(8)#5	2.335(10)
Cu(4)-N(1)#2	1.895(13)
Cu(4)-N(1)	1.895(13)
Cu(4)-O(4)	1.923(9)
Cu(4)-O(4)#2	1.923(9)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2 #2 -x,-y+1,-z+1 #3 -x,y-1/2,-z+3/2

#4 -x,-y,-z+1 #5 -x-1,-y,-z+1 #6 -x,y+1/2,-z+3/2

#7 x,-y+1/2,z-1/2 #8 -x-1,y+1/2,-z+1/2 #9 -x-1,y-1/2,-z+1/2