Supplementary Material (ESI) for CrystEngComm

Support Information

Isomorphic polysupramolecules assembled from mixvalent Cu-triazolate sheets, benzene-1,3,5-tricarboxylates and halides

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Table S1. Crystal data and structure refinement information for **1** and **2**

	1	**2**
Empirical formula	$C_{17}H_{11}BrCu_6N_{12}O_6$	$C_{17}H_{11}ClCu_6N_{12}O_6$
Formula weight	940.58	896.13
Crystal system	Tetragonal	Tetragonal
Space group	*I 4/m*	*P4/ncc*
a/ Å	20.3711(5)	20.321(2)
b/ Å	20.3711(5)	20.321(2)
c/ Å	13.7711(8)	13.6990(10)
α/°	90	90
β/°	90	90
γ/°	90	90
V/Å^3	5714.8(4)	5656.9(6)
Z	8	8
μ/mm^{-1}	5.839	4.581
Reflections collected	17794	27321
Unique reflections	3419	2498
Obsreflections [I>2σ(I)]	2588	1408
Rint	0.0295	0.0728
R1 [I >2σ(I)]	0.0366	0.0600
wR2 [I >2σ(I)]	0.0963	0.1533
Goodness-of-fit	1.138	1.096

Table S2. Selected bond lengths (Å) and angles (°) for **1**.

Br(1)-Cu(1)	2.9726(10)	Cu(3)-N(6)#2	1.887(6)
Cu(1)-N(3)#1	1.887(5)	Cu(3)-N(5)	1.890(6)
Cu(1)-N(1)	1.898(6)	N(3)-Cu(1)#3	1.887(5)
Cu(2)-N(4)	1.873(7)	N(6)-Cu(3)#4	1.887(6)
Cu(2)-N(2)	1.879(7)	C(8)-N(3)-Cu(1)#3	131.7(5)
N(3)#1-Cu(1)-N(1)	155.7(2)	N(1)-N(3)-Cu(1)#3	122.8(4)
N(3)#1-Cu(1)-Br(1)	99.84(16)	C(10)-N(4)-Cu(2)	129.5(5)
N(1)-Cu(1)-Br(1)	100.36(17)	C(9)-N(4)-Cu(2)	127.1(6)
N(4)-Cu(2)-N(2)	165.76(16)	C(9)-N(5)-Cu(3)	131.1(5)
N(6)#2-Cu(3)-N(5)	155.7(2)	N(6)-N(5)-Cu(3)	122.3(5)
C(7)-N(1)-Cu(1)	130.6(6)	C(10)-N(6)-Cu(3)#4	130.8(5)
N(3)-N(1)-Cu(1)	122.9(4)	N(5)-N(6)-Cu(3)#4	123.4(5)
C(8)-N(2)-Cu(2)	131.3(6)	C(7)-N(2)-Cu(2)	126.6(6)

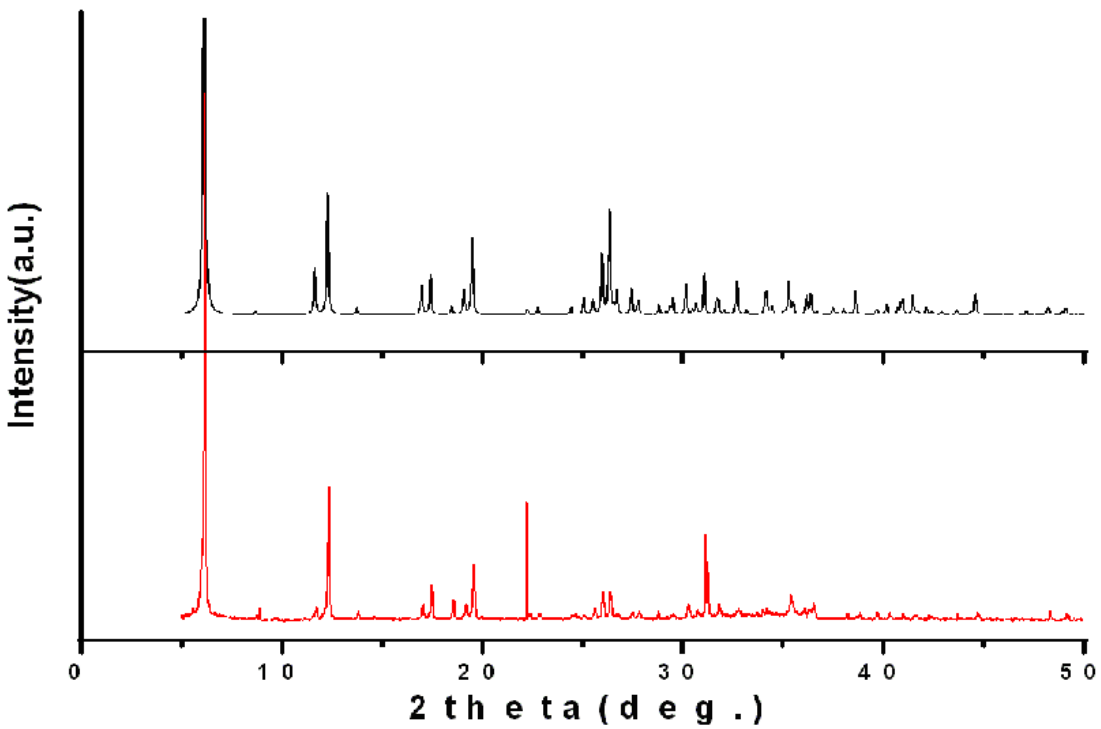
Symmetry transformations used to generate equivalent atoms: #1 -y,x,z #2 -y+1,x,z #3 y,-x,z #4 y,-x+1,z #5 x,y,-z

Table S3. Selected bond lengths (Å) and angles (°) for **2**.

Cu(1)-N(1)	1.880(6)	Cl(1)-Cu(1)#4	2.662(2)
Cu(1)-N(2)#1	1.888(6)	Cl(1)-Cu(1)#1	2.662(2)
Cu(1)-Cl(1)	2.662(3)	Cl(1)-Cu(1)#5	2.662(2)
Cu(2)-N(4)	1.876(7)	Cl(2)-Cu(3)#6	2.677(3)
Cu(2)-N(3)	1.882(7)	Cl(2)-Cu(3)#7	2.677(3)
Cu(2)-O(2)#2	2.43(5)	Cl(2)-Cu(3)#3	2.677(3)
Cu(3)-N(5)	1.887(6)	N(2)-Cu(1)#5	1.888(6)
Cu(3)-N(6)#3	1.889(6)	N(6)-Cu(3)#6	1.889(6)
Cu(3)-Cl(2)	2.677(3)	O(2)-Cu(2)#2	2.43(5)
N(1)-Cu(1)-N(2)#1	154.6(3)	Cu(3)-Cl(2)-Cu(3)#7	127.5(2)
N(1)-Cu(1)-Cl(1)	102.82(19)	Cu(3)#6-Cl(2)-Cu(3)#3	127.5(2)
N(2)#1-Cu(1)-Cl(1)	102.3(2)	Cu(3)-Cl(2)-Cu(3)#3	78.71(8)
N(4)-Cu(2)-N(3)	166.6(3)	Cu(3)#7-Cl(2)-Cu(3)#3	78.71(8)
N(4)-Cu(2)-O(2)#2	99.5(9)	C(1)-N(1)-Cu(1)	132.2(5)
N(3)-Cu(2)-O(2)#2	93.8(9)	N(2)-N(1)-Cu(1)	122.1(5)
N(5)-Cu(3)-N(6)#3	154.2(3)	C(2)-N(2)-Cu(1)#5	130.1(6)
N(5)-Cu(3)-Cl(2)	103.0(2)	N(1)-N(2)-Cu(1)#5	123.3(5)
N(6)#3-Cu(3)-Cl(2)	102.5(2)	C(1)-N(3)-Cu(2)	130.7(6)
Cu(1)#4-Cl(1)-Cu(1)#1	79.35(8)	C(2)-N(3)-Cu(2)	127.0(6)
Cu(1)#4-Cl(1)-Cu(1)#5	79.35(8)	C(3)-N(4)-Cu(2)	128.5(6)
Cu(1)#1-Cl(1)-Cu(1)#5	129.1(2)	C(4)-N(4)-Cu(2)	128.6(6)
Cu(1)#4-Cl(1)-Cu(1)	129.1(2)	C(3)-N(5)-Cu(3)	133.4(6)
Cu(1)#1-Cl(1)-Cu(1)	79.35(8)	N(6)-N(5)-Cu(3)	122.0(5)
Cu(1)#5-Cl(1)-Cu(1)	79.35(8)	C(4)-N(6)-Cu(3)#6	131.6(5)
Cu(3)#6-Cl(2)-Cu(3)	78.71(8)	N(5)-N(6)-Cu(3)#6	123.0(5)
Cu(3)#6-Cl(2)-Cu(3)#7	78.71(8)	C(11)-O(2)-Cu(2)#2	125.0(3)

Symmetry transformations used to generate equivalent atoms: #1 -y+3/2, x, z #2 y-1/2, x+1/2, -z+1/2 #3 -y+3/2, x+1, z #4 -x+3/2, -y+3/2, z #5 y, -x+3/2, z #6 y-1, -x+3/2, z #7 -x+1/2, -y+5/2, z

Fig. S1. Simulated (black) and experimental (red) XRD spectra for **1** (upper) and **2** (lower)



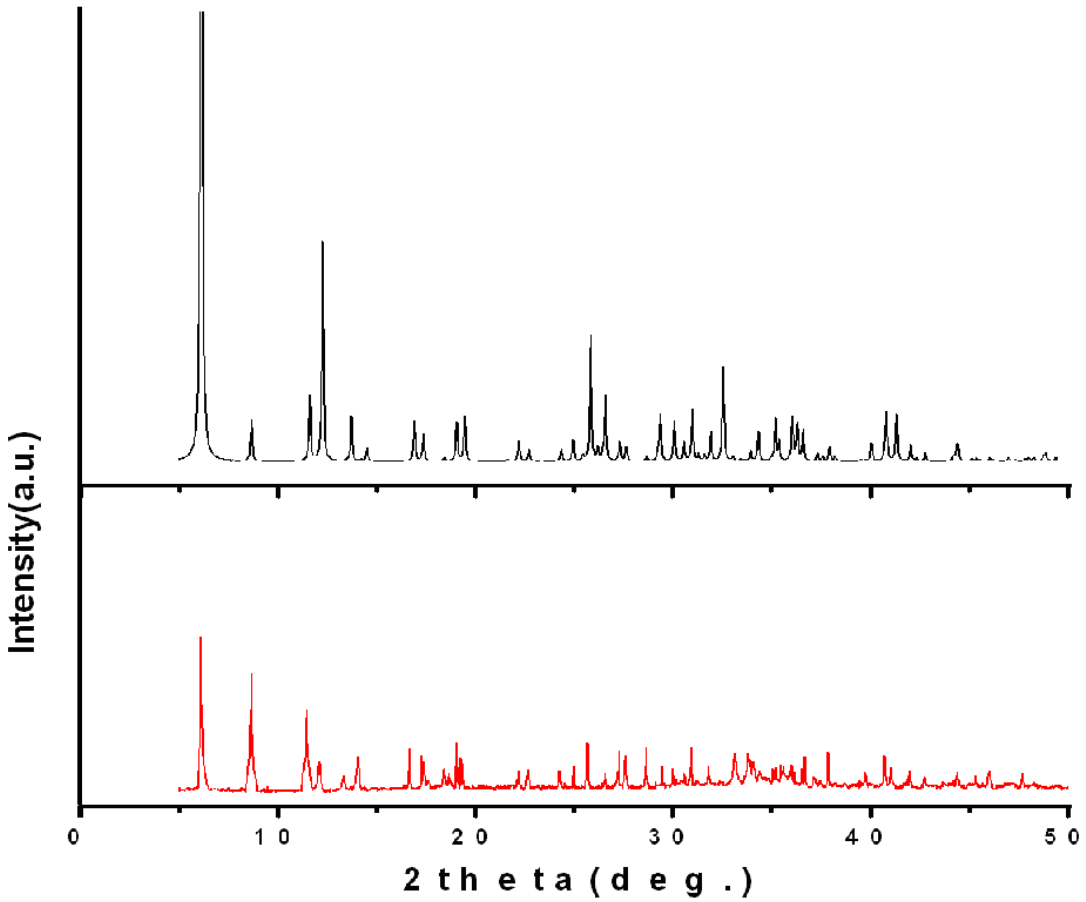


Fig. S2. XPS of **1**, evidencing the presence of Cu^{I} and Cu^{II}

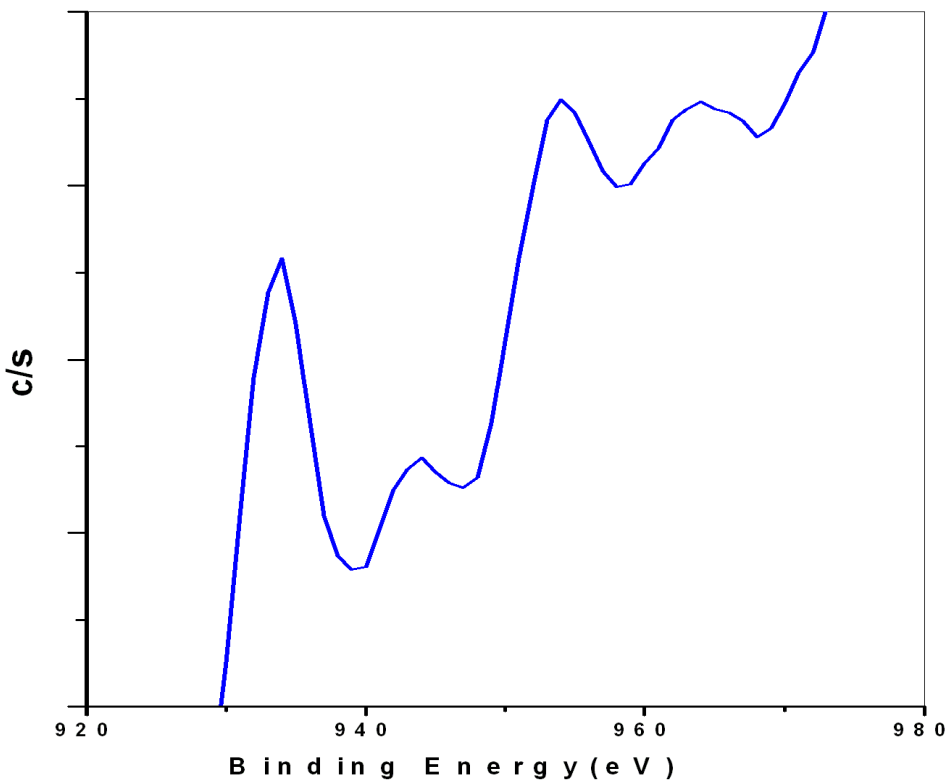


Fig. S3. Drawings showing the thermodynamic disorder of btc groups in **2** about (-1/3, 1/3, 0) plane due to the energy degeneracy of two states

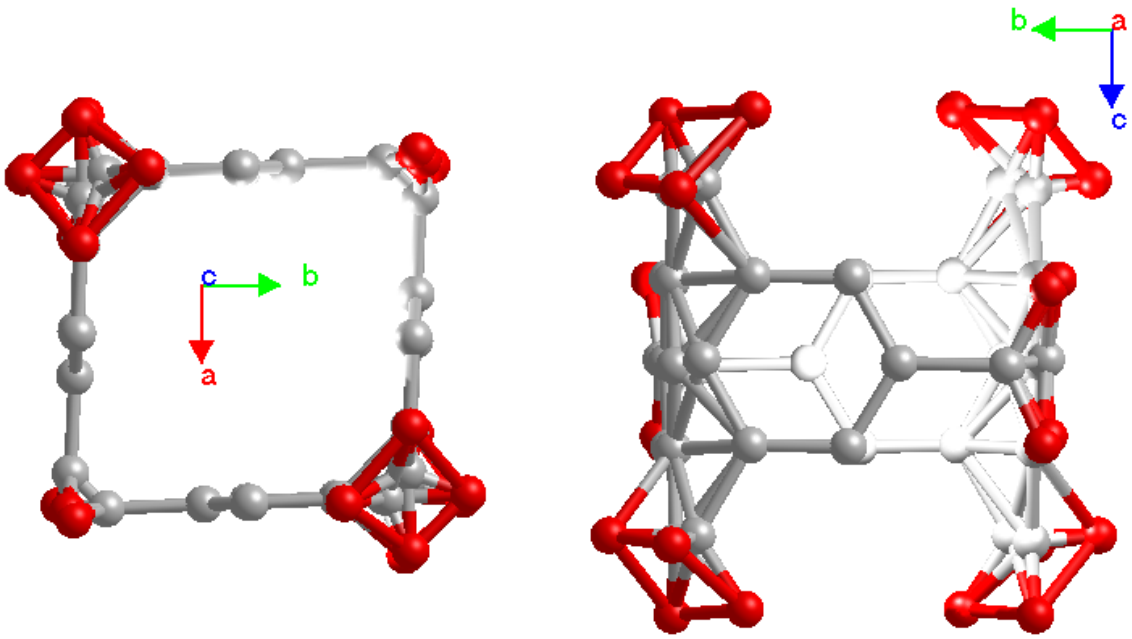


Fig. S4. The differential thermal analysis results of **1** (pink) and **2** (blue)