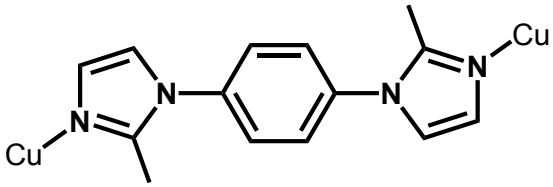
Supporting Informations

Effects of Hydroxy Substitutents on Cu(II) Coordination Polymers Based on 5-Hydroxyisophthalate Derivatives and 1,4-Bis(2-methylimidazol-1-yl)benzene

Yanqing Su,[a,b] Xinxiong Li, [b] Xiaoju Li,[a,b] Hui Pan[a,b] and Ruihu Wang*[b]

[a] *College of Materials Science and Engineering, Fujian Normal University, Fuzhou, Fujian, 350007, P. R. China.*

[b] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, P. R. China.*



Scheme S1 The coordination mode of bmib.

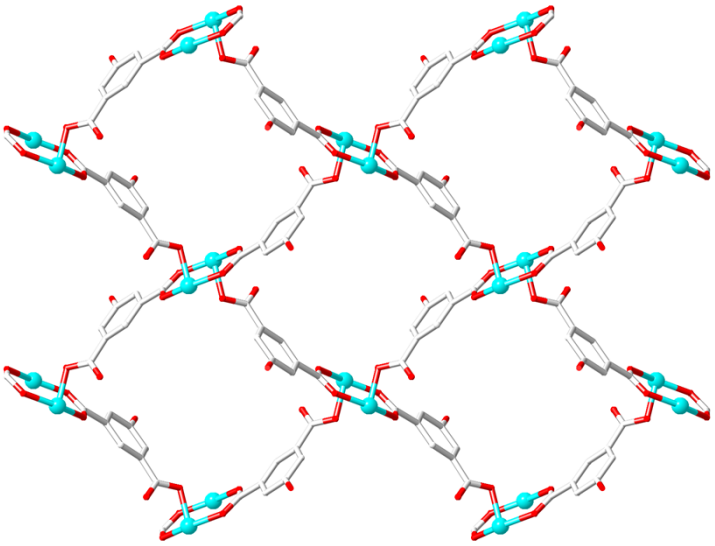


Figure S1 View of 2-D $[Cu_2(HO\text{-}ip)_2]_n$ layer containing square-shaped cavities in complex **1**.

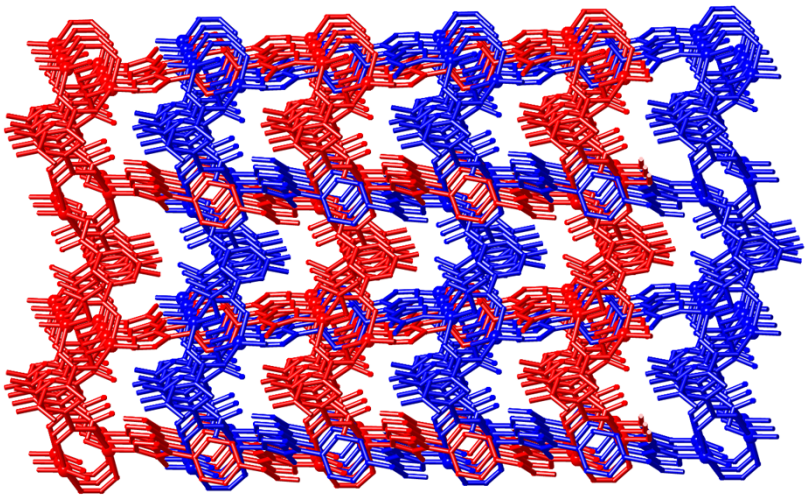


Figure S2 View of two-fold interpenetrating network in complex **1**.

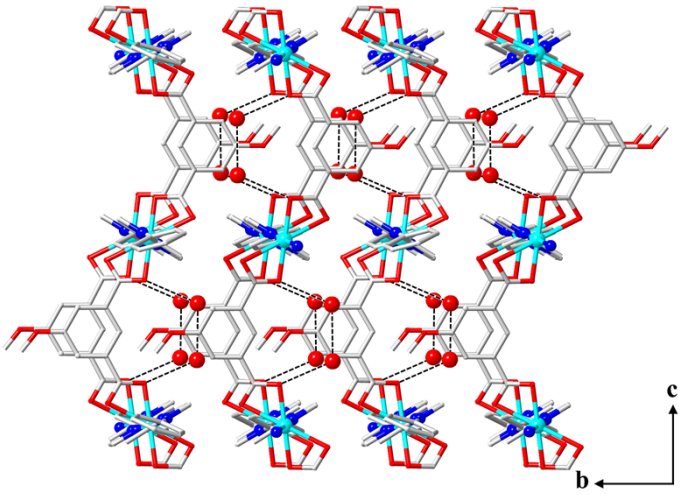


Figure S3 View of 3-D supramolecular network along the *a* axis in complex **3**.

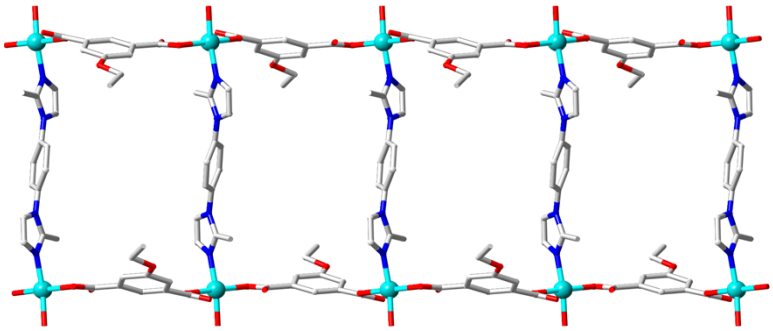


Figure S4 View of pillared-bichain in complex **4**.

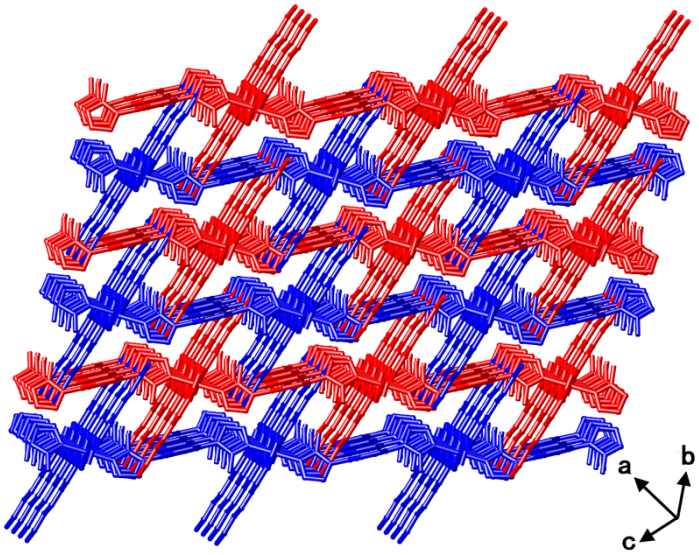


Figure S5 View of 2-D layer in complex **5**.

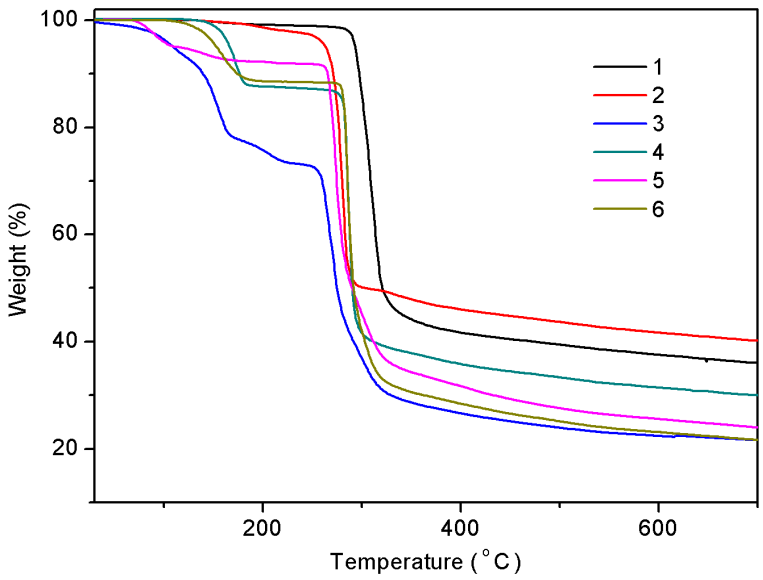
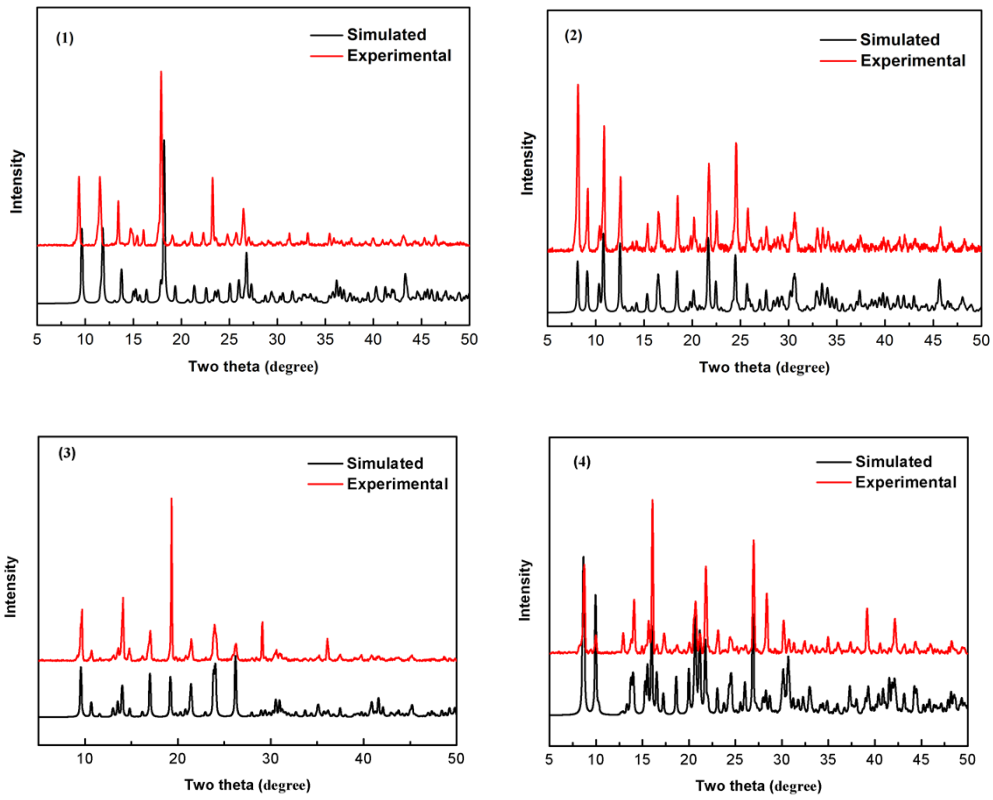


Figure S6 TGA curves of complexes **1**-**6**.



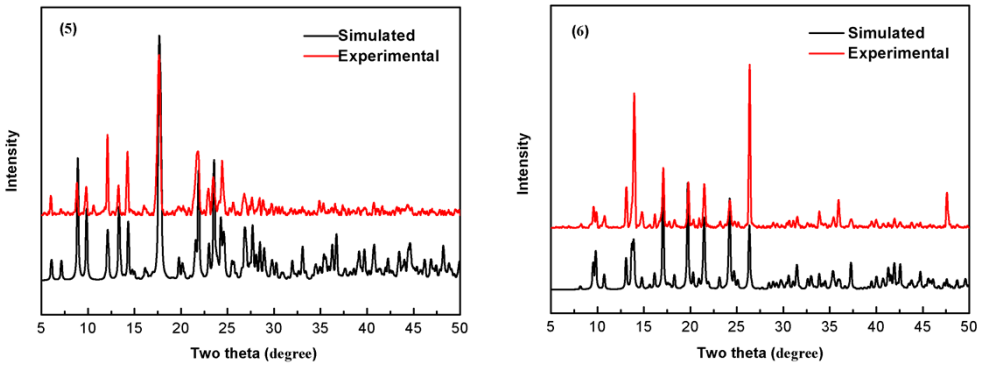


Figure S7 The simulated and experimental XRD patterns of complexes **1-6**.

Table S1. Selected bond lengths (Å) and Angles (°) for **1-6**.

		1	
Cu(1)-O(4)#1	1.9488(15)	Cu(1)-O(1)	1.9516(16)
Cu(1)-N(1)	1.9633(19)	Cu(1)-O(2)#2	1.9667(16)
Cu(1)-Cu(1)#2	2.8538(5)		
O(4)#1-Cu(1)-O(1)	89.94(7)	O(4)#1-Cu(1)-N(1)	163.26(8)
O(1)-Cu(1)-N(1)	97.11(7)	O(4)#1-Cu(1)-O(2)#2	87.37(7)
O(1)-Cu(1)-O(2)#2	160.60(7)	N(1)-Cu(1)-O(2)#2	90.79(8)
		2	
Cu(1)-O(9)	1.9339(19)	Cu(1)-N(1)	1.979(2)
Cu(1)-O(1)	2.0109(18)	Cu(1)-O(3)#1	2.045(2)
Cu(1)-O(6)	2.245(2)	Cu(2)-O(4)#2	1.9364(19)
Cu(2)-O(9)	1.9407(18)	Cu(2)-O(7)#3	1.949(2)
Cu(2)-O(2)	2.0011(19)	Cu(2)-O(9)#3	2.1699(19)
Cu(2)-Cu(2)#3	3.0455(10)		
O(9)-Cu(1)-N(1)	172.13(9)	O(9)-Cu(1)-O(1)	91.56(7)

N(1)-Cu(1)-O(1)	88.87(8)	O(9)-Cu(1)-O(3)#1	90.25(7)
N(1)-Cu(1)-O(3)#1	85.86(8)	O(1)-Cu(1)-O(3)#1	153.19(8)
O(9)-Cu(1)-O(6)	98.74(8)	N(1)-Cu(1)-O(6)	88.99(9)
O(1)-Cu(1)-O(6)	97.72(9)	O(3)#1-Cu(1)-O(6)	108.43(9)
O(4)#2-Cu(2)-O(9)	179.14(8)	O(4)#2-Cu(2)-O(7)#3	91.50(10)
O(9)-Cu(2)-O(7)#3	89.36(9)	O(4)#2-Cu(2)-O(2)	86.01(9)
O(9)-Cu(2)-O(2)	93.34(9)	O(7)#3-Cu(2)-O(2)	137.81(9)
O(4)#2-Cu(2)-O(9)#3	95.17(7)	O(9)-Cu(2)-O(9)#3	84.55(7)
O(7)#3-Cu(2)-O(9)#3	110.28(8)	O(2)-Cu(2)-O(9)#3	111.89(8)

3

Cu(1)-N(1)	1.9805(19)	Cu(1)-O(2)	2.412(2)
Cu(1)-O(1)	2.084(2)		
N(1)-Cu(1)-O(2)	89.39(8)	N(1)-Cu(1)-O(1)#1	88.87(8)
O(1)#1-Cu(1)-O(2)	122.23(8)	N(1)-Cu(1)-O(1)	91.13(8)
N(1)-Cu(1)-O(2)#1	90.61(8)	O(1)-Cu(1)-O(2)	57.78(8)
N(1)-Cu(1)-N(1)#1	180.0	O(1)-Cu(1)-O(1)#1	180.0(1)

4

Cu(1)-O(3)#1	1.9576(14)	Cu(1)-O(1W)	1.9587(15)
Cu(1)-O(2)	1.9873(13)	Cu(1)-N(1)	1.9893(18)
O(3)-Cu(1)#2	1.9577(14)		
O(3)#1-Cu(1)-O(1W)	89.40(6)	O(2)-Cu(1)-N(1)	90.32(6)
O(1W)-Cu(1)-O(2)	90.11(6)	O(3)#1-Cu(1)-N(1)	90.81(6)
O(1W)-Cu(1)-N(1)	168.22(6)	O(3)#1-Cu(1)-O(2)	176.79(5)

5

Cu(1)-O(1)	1.982(2)	Cu(2)-O(4)	1.953(2)
Cu(1)-N(1)	1.982(3)	Cu(2)-N(4)#3	2.006(3)
O(1)-Cu(1)-O(1)#1	179.999(1)	O(1)-Cu(1)-N(1)	87.69(12)
O(1)#1-Cu(1)-N(1)	92.31(12)	N(1)-Cu(1)-N(1)#1	180.00(8)
O(4)-Cu(2)-N(4)#4	89.26(11)	O(4)-Cu(2)-N(4)#3	90.74(11)
N(4)#3-Cu(2)-N(4)#4	180.00(15)	O(4)#2-Cu(2)-O(4)	179.999(1)
		6	
Cu(1)-N(1)	1.978(2)	Cu(1)-O(1)	2.004(2)
N(1)-Cu(1)-O(1)	90.00(7)	N(1)-Cu(1)-O(1)#1	89.99(7)
N(1)-Cu(1)-N(1)#1	180.0	O(1)-Cu(1)-O(1)#1	180.0

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

Table S2 Bond Valence Sums analysis for complex **1**

Assume Valence = 1 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
Nr	Bond	Dist	R	B	BVal	Sum	Diff - Source
1	Cu(1)-O(4A)	1.9488	1.6100	0.37	0.400	0.400	0.600 -
2	Cu(1)-O(1)	1.9515	1.6100	0.37	0.397	0.798	0.202 -
3	Cu(1)-N(1)	1.9630	1.5200	0.37	0.302	1.100	0.100 -
4	Cu(1)-O(2C)	1.9666	1.6100	0.37	0.381	1.481	0.481 -
5	Cu(1)-O(4F)	2.5301	1.6100	0.37	0.083	1.564	0.564 -
6	Cu(1)-O(3A)	2.6804	1.6100	0.37	0.055	**1.620**	**0.620 -**

Assume Valence = 2 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
Nr	Bond	Dist	R	B	BVal	Sum	Diff - Source
1	Cu(1)-O(4A)	1.9488	1.6790	0.37	0.482	0.482	1.518 -
2	Cu(1)-O(1)	1.9515	1.6790	0.37	0.479	0.961	1.039 -
3	Cu(1)-N(1)	1.9630	1.7510	0.37	0.564	1.525	0.475 -
4	Cu(1)-O(2C)	1.9666	1.6790	0.37	0.460	1.985	0.015 -
5	Cu(1)-O(4F)	2.5301	1.6790	0.37	0.100	**2.085**	**0.085 -**
Assume Valence = 3 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
Nr	Bond	Dist	R	B	BVal	Sum	Diff - Source
1	Cu(1)-O(4A)	1.9488	1.7350	0.37	0.561	0.561	2.439 -
2	Cu(1)-O(1)	1.9515	1.7350	0.37	0.557	1.11	1.882 -
3	Cu(1)-N(1)	1.9630	1.7680	0.37	0.590	1.708	1.292 -
4	Cu(1)-O(2C)	1.9666	1.7350	0.37	0.535	2.243	0.757 -

Table S3 Bond valence sums analysis for complex **2**

Cu(1)							
Assume Valence = 1 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
Nr	Bond	Dist	R	B	BVal	Sum	Diff - Source
1	Cu(1)-O(9)	1.9340	1.6100	0.37	0.417	0.417	0.583 -
2	Cu(1)-N(1)	1.9790	1.5200	0.37	0.289	0.706	0.294 -
3	Cu(1)-O(1)	2.0110	1.6100	0.37	0.338	1.044	0.044 -
4	Cu(1)-O(3D)	2.0450	1.6100	0.37	0.309	1.353	0.353 -
5	Cu(1)-O(6)	2.2450	1.6100	0.37	0.180	**1.532**	**0.532 –**
Assume Valence = 2 -- Min. Bond Val Contribution = 0.04 * Cation Val.							

Nr	Bond	Dist	R	B	BVal	Sum	Diff - Source
1	Cu(1)-O(9)	1.9340	1.6790	0.37	0.502	0.502	1.498 -
2	Cu(1)-N(1)	1.9790	1.7510	0.37	0.540	1.042	0.958 -
3	Cu(1)-O(1)	2.0110	1.6790	0.37	0.408	1.450	0.550 -
4	Cu(1)-O(3D)	2.0450	1.6790	0.37	0.372	1.822	0.178 -
5	Cu(1)-O(6)	2.0450	1.6790	0.37	0.217	**2.038**	**0.038 –**
Assume Valence = 3 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
1	Cu(1)-O(9)	1.9340	1.7350	0.37	0.584	0.584	2.416 -
2	Cu(1)-N(1)	1.9790	1.7680	0.37	0.565	1.149	1.851 -
3	Cu(1)-O(1)	2.0110	1.7350	0.37	0.474	1.624	1.376 -
4	Cu(1)-O(3D)	2.0450	1.7350	0.37	0.433	2.056	0.944 -
5	Cu(1)-O(6)	2.0450	1.7350	0.37	0.252	**2.308**	**0.692 –**
Cu(2)							
Assume Valence = 1 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
1	Cu(2)-O(4G)	1.9360	1.6100	0.37	0.414	0.414	0.586 -
2	Cu(2)-O(9)	1.9410	1.6100	0.37	0.409	0.823	0.177 -
3	Cu(2)-O(7H)	1.9490	1.6100	0.37	0.400	1.223	0.223 -
4	Cu(2)-O(2)	2.0010	1.6100	0.37	0.348	1.571	0.571 -
5	Cu(2)-O(9H)	2.1700	1.6100	0.37	0.220	**1.791**	**0.791 –**
Assume Valence = 2 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
1	Cu(2)-O(4G)	1.9360	1.6790	0.37	0.499	0.499	1.501 -
2	Cu(2)-O(9)	1.9410	1.6790	0.37	0.493	0.992	1.008 -
3	Cu(2)-O(7H)	1.9490	1.6790	0.37	0.482	1.474	0.526 -
4	Cu(2)-O(2)	2.0010	1.6790	0.37	0.419	1.893	0.107 -

5	Cu(2)-O(9H)	2.1700	1.6790	0.37	0.265	**2.158**	**0.158 -**
Assume Valence = 3 -- Min. Bond Val Contribution = 0.04 * Cation Val.							
1	Cu(2)-O(4G)	1.9360	1.7350	0.37	0.581	0.581	2.419 -
2	Cu(2)-O(9)	1.9410	1.7350	0.37	0.573	1.154	1.846 -
3	Cu(2)-O(7H)	1.9490	1.7350	0.37	0.561	1.715	1.285 -
4	Cu(2)-O(2)	2.0010	1.7350	0.37	0.487	2.202	0.798 -
5	Cu(2)-O(9H)	2.1700	1.7350	0.37	0.309	**2.511**	**0.489 -**