Supporting Information

Solvent-Induced Deviation in Square-Grid Layers of Microporous Cu(II) Isophthalates: Layer Stacking and Gas Adsorption Properties

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Table 1S *Bond Distances (Å) and Angles (deg) of Metal Coordination in Complexes* ***1-5***

		1	
Cu(1)-O(2)	1.962(2)	Cu(1)-O(1)#2	1.967(2)
Cu(1)-O(1W)	2.124(3)	Cu(1)-Cu(1)#3	2.6130(9)
O(2)#1-Cu(1)-O(2)	88.21(15)	O(2)-Cu(1)-O(1)#3	168.34(9)
O(2) #1-Cu(1)-O(1)#3	89.60(12)	O(1)#2-Cu(1)-O(1)#3	90.25(18)
O(2)-Cu(1)-O(1W)	93.71(9)	O(1)#2-Cu(1)-O(1W)	97.86(9)
O(2)-Cu(1)-Cu(1)#3	81.72(7)	O(1)#2-Cu(1)-Cu(1)#3	86.63(7)
O(1W)-Cu(1)-Cu(1)#3	173.60(10)		
		2	
Cu(1)-O(2)	1.961(6)	Cu(1)-O(1)#2	1.966(6)
Cu(1)-O(3)	2.139(8)	Cu(1)-Cu(1)#3	2.604(2)
O(2)-Cu(1)-O(2)#1	90.8(5)	O(2)-Cu(1)-O(1)#2	89.2(3)
O(2)-Cu(1)-O(1)#3	168.4(3)	O(1)#2-Cu(1)-O(1)#3	88.4(4)
O(2)-Cu(1)-O(3)	97.8(2)	O(1)#2-Cu(1)-O(3)	93.8(2)
O(2)-Cu(1)-Cu(1)#3	86.44(19)	O(1)#2-Cu(1)-Cu(1)#3	81.93(18)
O(3)-Cu(1)-Cu(1)#3	174.0(2)		
		3	

Cu(1)-O(1)	1.945(11)	Cu(1)-O(3)#2	1.955(11)
Cu(1)-O(7)#1	1.953(12)	Cu(1)-O(5)	1.956(11)
Cu(1)-O(1W)	2.166(3)	Cu(1)-Cu(2)	2.616(3)
Cu(2)-O(8)#1	1.923(11)	Cu(2)-O(2)	1.958(11)
Cu(2)-O(6)	1.962(11)	Cu(2)-O(4)#2	1.966(11)
Cu(2)-O(9)	2.166(13)		
O(1)-Cu(1)-O(3)#2	167.9(5)	O(1)-Cu(1)-O(7)#1	89.7(5)
O(3)#2-Cu(1)-O(7)#1	88.8(5)	O(1)-Cu(1)-O(5)	91.5(5)
O(3)#2-Cu(1)-O(5)	87.6(5)	O(7)#1-Cu(1)-O(5)	168.3(5)
O(1)-Cu(1)-O(1W)	87.4(5)	O(3)#2-Cu(1)-O(1W)	104.7(5)
O(7)#1-Cu(1)-O(1W)	91.6(5)	O(5)-Cu(1)-O(1W)	100.1(5)
O(1)-Cu(1)-Cu(2)	80.4(4)	O(3)#2-Cu(1)-Cu(2)	87.5(4)
O(7)#1-Cu(1)-Cu(2)	80.4(4)	O(5)-Cu(1)-Cu(2)	88.3(4)
O(1W)-Cu(1)-Cu(2)	165.3(3)	O(8)#1-Cu(2)-O(2)	87.9(5)
O(8)#1-Cu(2)-O(6)	167.2(5)	O(2)-Cu(2)-O(6)	92.3(5)
O(8)#1-Cu(2)-O(4)#2	88.4(5)	O(2)-Cu(2)-O(4)#2	169.3(5)
O(6)-Cu(2)-O(4)#2	89.1(5)	O(8)#1-Cu(2)-O(9)	101.0(5)
O(2)-Cu(2)-O(9)	93.3(5)	O(6)-Cu(2)-O(9)	91.7(5)

O(4)#2-Cu(2)-O(9)	97.2(5)	O(8)#1-Cu(2)-Cu(1)	87.5(42)
O(2)-Cu(2)-Cu(1)	88.6(3)	O(6)-Cu(2)-Cu(1)	79.8(3)
O(4)#1-Cu(2)-Cu(1)	81.3(3)	O(9)-Cu(2)-Cu(1)	171.4(4)

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Cu(1)-O(4)#1	1.953(6)	Cu(1)-O(8)#2	1.963(6)
Cu(1)-O(7)#3	1.988(6)	Cu(1)-O(3)	1.991(5)
Cu(1)-O(9)	2.127(7)	Cu(1)-Cu(1)#1	2.6404(18)
Cu(2)-O(6)	1.966(5)	Cu(2)-O(2)	1.980(5)
Cu(2)-O(1W)	2.141(8)	Cu(2)-Cu(3)	2.6494(18)
Cu(3)-O(1)	1.940(5)	Cu(3)-O(5)	1.969(5)
Cu(3)-O(11)	2.094(9)		
O(4)#1-Cu(1)-O(8)#2	170.3(3)	O(4)#1-Cu(1)-O(7)#3	90.0(3)
O(8)#2-Cu(1)-O(7)#3	89.4(3)	O(4)#1-Cu(1)-O(3)	88.7(2)
O(8)#2-Cu(1)-O(3)	89.5(3)	O(7)#3-Cu(1)-O(3)	165.7(3)
O(4)#1-Cu(1)-O(9)	95.8(3)	O(8)#2-Cu(1)-O(9)	93.8(3)
O(7)#3-Cu(1)-O(9)	103.1(3)	O(3)-Cu(1)-O(9)	91.2(2)
O(4)#1-Cu(1)-Cu(1)#1	86.97(18)	O(8)#2-Cu(1)-Cu(1)#1	83.36(18)
O(7)#3-Cu(1)-Cu(1)#1	84.54(18)	O(3)-Cu(1)-Cu(1)#1	81.16(17)

O(9)-Cu(1)-Cu(1)#1	171.83(19)	O(6)#4-Cu(2)-O(6)	91.8(4)
O(6)#4-Cu(2)-O(2)	167.4(3)	O(6)-Cu(2)-O(2)	87.7(2)
O(2)-Cu(2)-O(2)#4	90.1(3)	O(6)-Cu(2)-O(1W)	95.9(2)
O(2)-Cu(2)-O(1W)	96.7(3)	O(6)-Cu(2)-Cu(3)	81.89(17)
O(2)-Cu(2)-Cu(3)	85.59(18)	O(1W)-Cu(2)-Cu(3)	176.8(3)
O(1)-Cu(3)-O(1)#4	90.3(4)	O(1)-Cu(3)-O(5)#4	167.7(3)
O(1)-Cu(3)-O(5)	88.2(3)	O(5)#4-Cu(3)-O(5)	90.7(4)
O(1)-Cu(3)-O(11)	95.3(3)	O(5)-Cu(3)-O(11)	96.9(2)
O(1)-Cu(3)-Cu(2)	81.88(19)	O(5)-Cu(3)-Cu(2)	85.86(17)
O(11)-Cu(3)-Cu(2)	176.0(2)		

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Cu(1)-O(2)#1	1.954(3)	Cu(1)-O(1)	1.959(3)
Cu(1)-O(6)#1	1.969(3)	Cu(1)-O(5)	1.980(3)
Cu(1)-N(1)	2.206(4)	Cu(1)-Cu(1)#1	2.6469(11)
Cu(2)-O(8)	1.964(3)	Cu(2)-O(7)#3	1.969(3)
Cu(2)-O(1W)	2.147(5)	Cu(2)-Cu(2)#3	2.6193(15)
Cu(3)-O(4)	1.953(4)	Cu(3)-O(3)#5	1.954(4)
Cu(3)-O(2W)	2.211(7)	Cu(3)-Cu(3)#5	2.6429(16)

O(2)#1-Cu(1)-O(1)	167.92(14)	O(2)#1-Cu(1)-O(6)#1	89.50(15)
O(1)-Cu(1)-O(6)#1	88.22(15)	O(2)#1-Cu(1)-O(5)	88.14(15)
O(1)-Cu(1)-O(5)	91.61(14)	O(6)#1-Cu(1)-O(5)	167.85(13)
O(2)#1-Cu(1)-N(1)	101.49(15)	O(1)-Cu(1)-N(1)	90.55(15)
O(6)#1-Cu(1)-N(1)	96.47(15)	O(5)-Cu(1)-N(1)	95.68(15)
O(2)#1-Cu(1)-Cu(1)#1	87.74(10)	O(1)-Cu(1)-Cu(1)#1	80.28(10)
O(6)#1-Cu(1)-Cu(1)#1	86.70(10)	O(5)-Cu(1)-Cu(1)#1	81.31(10)
N(1)-Cu(1)-Cu(1)#1	170.23(12)	O(8)-Cu(2)-O(8)#2	90.1(2)
O(8)-Cu(2)-O(7)#3	168.69(14)	O(8)-Cu(2)-O(7)#4	88.46(15)
O(7)#3-Cu(2)-O(7)#4	90.8(2)	O(8)-Cu(2)-O(1W)	95.52(16)
O(3)#5-Cu(3)-O(3)#6	90.9(2)	O(7)#3-Cu(2)-O(1W)	95.79(16)
O(8)-Cu(2)-Cu(2)#3	84.40(10)	O(7)#3-Cu(2)-Cu(2)#3	84.29(10)
O(1W)-Cu(2)-Cu(2)#3	179.88(19)	O(4)#2-Cu(3)-O(4)	91.4(3)
O(4)#2-Cu(3)-O(3)#5	168.04(16)	O(4)-Cu(3)-O(3)#5	87.60(18)
O(4)-Cu(3)-O(2W)	94.9(2)	O(3)#5-Cu(3)-O(2W)	97.1(2)
O(4)-Cu(3)-Cu(3)#6	83.24(11)	O(3)#5-Cu(3)-Cu(3)#6	84.81(11)
O(2W)-Cu(3)-Cu(3)#6	177.3(3)		

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

5: #1 -*x*+3/2, -*y*+3/2, -*z*+2; #2 *x*, -*y*+1, *z*; #3 -*x*+1, -*y*+1, -*z*+1; #4 -*x*+1, *y*, -*z*+1; #5 -*x*+2, -*y*+1, -*z*+3; #6 -*x*+2, *y*, -*z*+3.

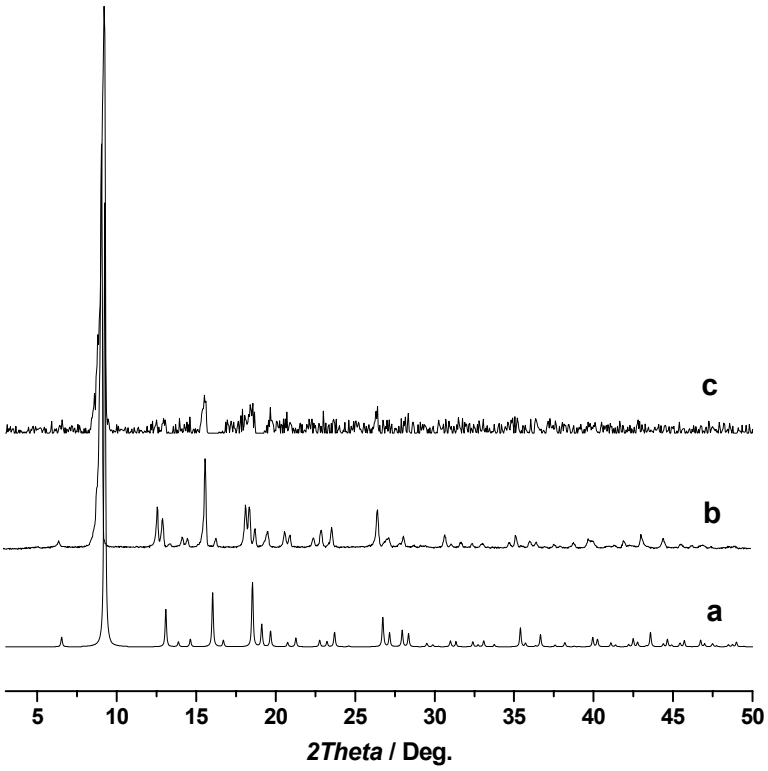

Figure 1S PXRD patterns of **1**: (a) simulated from crystallographic CIF file, (b) as made, and (c) after removal of the guest molecules.

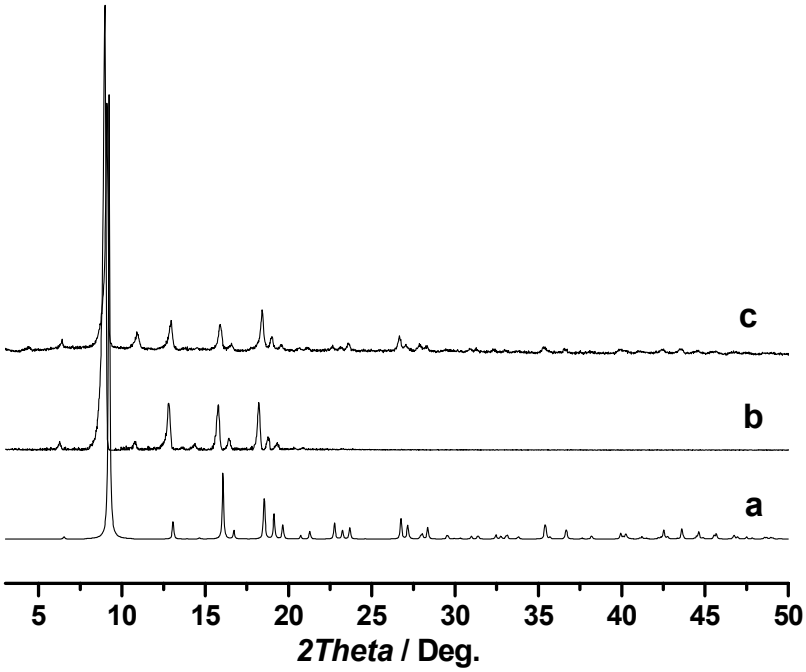

Figure 2S PXRD patterns of **2**: (a) simulated from crystallographic CIF file, (b) as made, and (c) after removal of the solvent molecules.

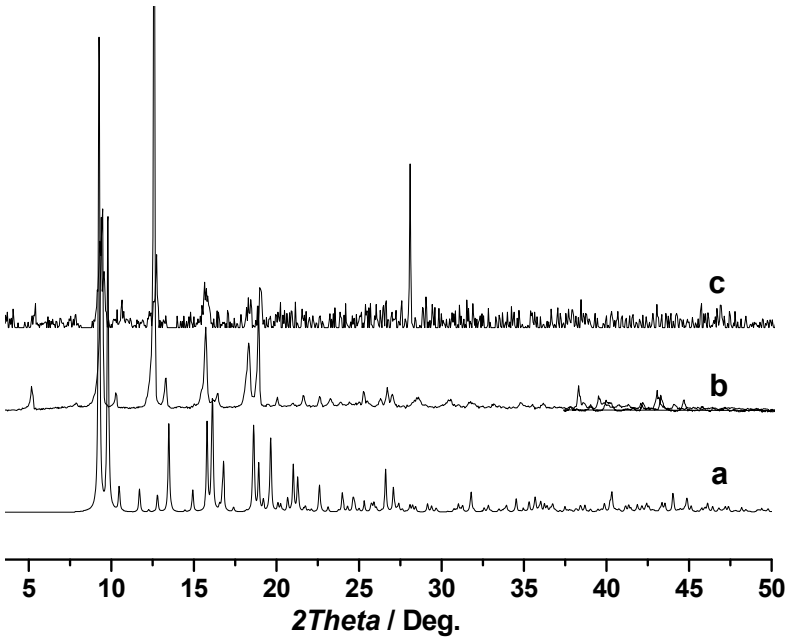

Figure 3S PXRD patterns of **3**: (a) simulated from crystallographic CIF file, (b) as made, and (c) after removal of the guest molecules.

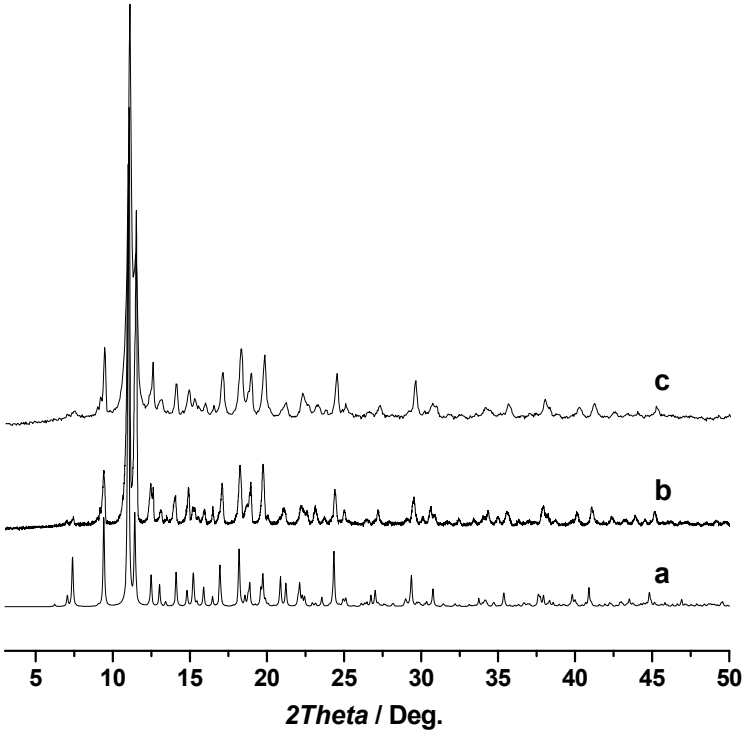

Figure 4S PXRD patterns of **4**: (a) simulated from crystallographic CIF file, (b) as made, and (c) after removal of the guest molecules.