Electronic Supplementary Material for CrystEngComm

Supporting Information for the paper titled **"Metal Disordering Cu(II) Supramolecular Isomers Constructed from a Tripodal Ligand Possessing Two Different Functional Groups"** to .*CrystEngComm.*

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Table S1. Selected bond lengths (Å) and angles (°) of **1** and **2**.

		Complex **1**	
Cu(1)–O(1A)	2.091(2)	O(3) –Cu(1)–O(1A)	108.09(9)
Cu(1)–O(2)	2.103(2)	O(3)–Cu(1)–O(2)	70.40(9)
Cu(1)–O(3)	2.412(2)	O(3)–Cu(1)–O(4)	93.48(12)
Cu(1)–O(4)	1.959(4)	O(3)–Cu(1)–N(1)	98.79(10)
Cu(1)–N(1)	2.065(3)	O(2)–Cu(1)–O(4)	83.40(12)
		O(4)–Cu(1)–O(1A)	80.84(12)
		O(1A)–Cu(1)–N(1)	100.76(11)
		N(1)–Cu(1)–O(2)	95.12(11)
		Complex **2**	
Cu(1)-O(1)	1.921(3)	O(1w)-Cu(1)-O(1)	89.26(11)
Cu(1)-N(1)	1.999(3)	O(1w)-Cu(1)-O(16)	89.77(11)
Cu(1)-O(3)	2.450(2)	O(1w)-Cu(1)-N(1)	171.10(13)
Cu(1)-O(1w)	1.920(3)	O(16)-Cu(1)-N(1)	89.92(11)
Cu(1)-O(16)	1.960(3)	O(1)-Cu(1)-O(16)	173.53(11)
Cu(2)-O(4)	1.990(3)	O(1)-Cu(1)-N(1)	92.02(11)
Cu(2)-N(2)	2.03(4)	C(32')-Cu(2)-O(2w)	169.3(16)
Cu(2)-O(2w)	1.988(2)	O(2w)-Cu(2)-O(4)	87.27(11)
Cu(3)-O(7)	1.980(3)	O(2w)-Cu(2)-N(2)	167.4(11)
Cu(3)-O(10)	1.959(3)	C(32')-Cu(2)-O(4)	94.9(16)
Cu(4)-O(2wE)	2.102(2)	O(4)-Cu(2)-N(2)	91.3(12)
Cu(5)-O(3wE)	1.922(3)	O(3w)-Cu(3)-O(10)	85.56(11)
Cu(5)-N(3')	2.149(6)	O(10)-Cu(3)-O(7)	172.30(12)
O(5)-Cu(5A)	2.257(3)	O(3w)-Cu(3)-N(3)	169.9(6)
O(6)-Cu(5A)	2.452(2)	O(7)-Cu(3)-N(3)	91.6(7)
O(9)-Cu(4B)	2.470(3)	O(3w)-Cu(3)-O(7)	88.54(11)
O(11)-Cu(4C)	2.292(3)	O(10)-Cu(3)-N(3)	95.0(7)
O(13)-Cu(2D)	2.233(3)	O(3w)-Cu(3)-O(12)	93.37(11)
O(14)-Cu(5C)	2.025(3)	O(7)-Cu(3)-O(12)	101.64(11)
O(15)-Cu(2D)	2.501(3)	N(3)-Cu(3)-O(12)	96.4(5)
		N(2')-Cu(4)-O(2wE)	177.2(2)
		O(3wE)-Cu(5)-N(3')	156.2(2)

Symmetry codes: for **1**, A: 1 + *y*, 1 – *x* + *y*, - *z*; for **2**, A: 1 + *y*, 1 – *x* + *y*, 1 - *z*; B: 2 - *x*, 1 - *y*, 1 - *z*; C: + *x* - *y*, -1 + *x*, 1 - *z*; D: 1 – *x* + *y*, 1 - *x*, + *z*; E: + *x*, + *y*, 1 + *z*.

Figure S1. Three-dimensional network of **1** viewed down the *b* (bottom) axis, respectively, showing space-filling of the solvent molecules. (Red, oxygen) Hydrogen atoms are omitted for clarity.

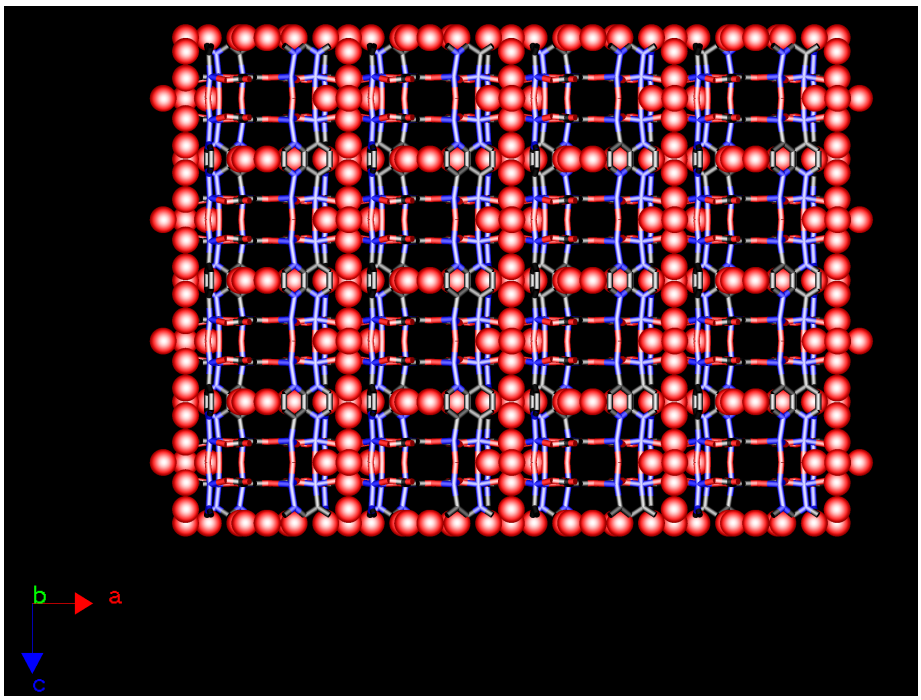

Figure S2. Three-dimensional network of **2** viewed down the *b* axis, respectively, showing the space-filling of the solvent molecules. (Red, oxygen; white, carbon; blue, nitrogen.) Hydrogen atoms are omitted for clarity.

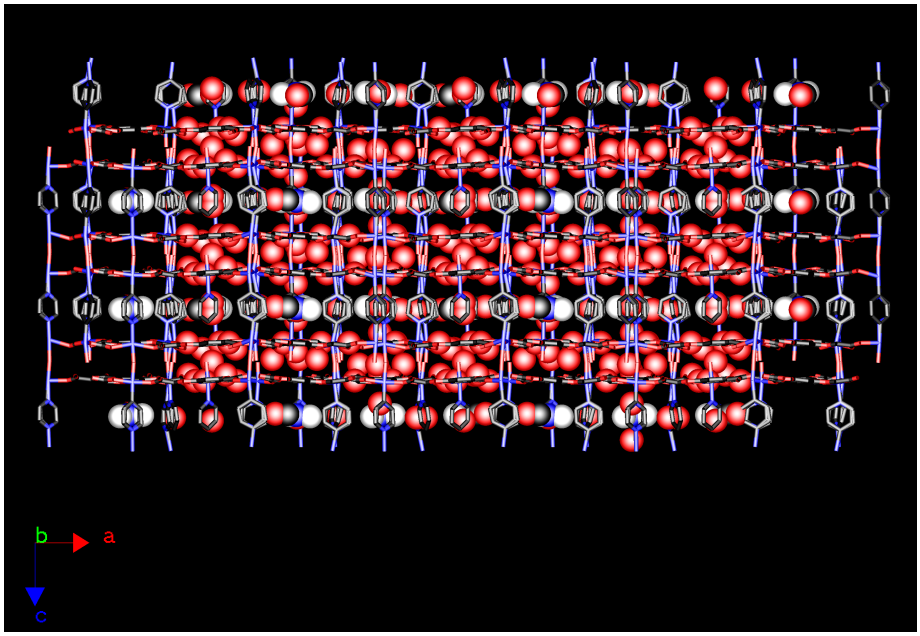

Figure S3. TGA of **1** (top) and **2** (bottom).