Electronic Supplementary Material (ESI) for CrystEngComm

Structural versatile of seven copper(II) coordination polymers constructed with long flexible ligand 1,4-bis(1,2,4-triazol-1-yl)butane

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Table S1 Selected bond lengths [Å] and angles [°] for 1-7

		1	
Cu(1)-N(3)	1.9854(19)	Cu(1)-O(1)	2.352(3)
Cu(1)-O(2)	2.341(3)	Cu(1)-O(3)	2.0182(18)
N(3)-Cu(1)-O(1)	89.35(5)	N(3)-Cu(1)-O(2)	90.65(5)
N(3)-Cu(1)-O(3)	88.31(8)	O(2)-Cu(1)-O(1)	180.000(1)
O(3)-Cu(1)-O(1)	87.44(5)	O(3)-Cu(1)-O(2)	92.56(5)
N(3)-Cu(1)-N(3A)	178.70(11)	N(3)-Cu(1)-O(3A)	91.63(8)
O(3)-Cu(1)-O(3A)	174.88(10)		
		2	
Cu(1)-N(3)	2.0359(17)	Cu(1)-N(6A)	2.0069(17)
Cu(1)-Cl(1)	2.8029(7)		
N(3)-Cu(1)-N(6A)	90.89(7)	N(3)-Cu(1)-Cl(1)	89.93(5)
N(6A)-Cu(1)-Cl(1)	91.89(5)		
		3	
Cu(1)-N(3)	1.9975(13)	Cu(1)-N(4)	1.9661(14)
Cu(1)-S(1B)	2.9878(7)		
N(3)-Cu(1)-N(4)	90.70(6)	N(3)-Cu(1)-S(1B)	88.48(4)
N(4)-Cu(1)-S(1C)	98.02(5)		
		4	
Cu(1)-N(3)	2.012(3)	Cu(1)-O(1)	2.407(4)

N(3)-Cu(1)-N(3A)	90.03(17)	N(3)-Cu(1)-N(3B)	175.92(15)
N(3)-Cu(1)-N(3C)	90.11(17)	O(1)-Cu(1)-O(1C)	180.0
N(3)-Cu(1)-O(1)	92.04(7)		
		5	
Cu(1)-N(3)	2.012(4)	Cu(1)-O(1)	2.400(5)
N(3)-Cu(1)-N(3A)	179.31(18)	N(3)-Cu(1)-N(3B)	90.2(2)
N(3)-Cu(1)-N(3C)	89.8(2)	O(1)-Cu(1)-O(1C)	180.0
N(3)-Cu(1)-O(1)	90.35(9)		
		6	
Cu(1)-O(1)	1.9685(17)	Cu(1)-N(3)	2.0034(19)
O(1)-Cu(1)-N(3)	90.64(8)	O(1A)-Cu(1)-N(3)	89.36(8)
		7	
Cu(1)-O(1)	2.196(3)	Cu(1)-O(5A)	1.943(3)
Cu(1)-O(7B)	2.019(3)	Cu(1)-O(9)	1.999(4)
Cu(1)-N(3)	1.980(4)	Cu(2)-O(2C)	1.954(3)
Cu(2)-O(3)	1.971(3)	Cu(2)-O(10)	2.002(3)
Cu(2)-O(11)	2.361(4)	Cu(2)-N(6)	2.001(4)
O(5A)-Cu(1)-O(1)	87.36(13)	O(7B)-Cu(1)-O(1)	96.41(15)
O(9)-Cu(1)-O(1)	106.2(2)	O(5A)-Cu(1)-O(7B)	88.20(12)
O(5A)-Cu(1)-O(9)	91.01(16)	O(9)-Cu(1)-O(7B)	157.32(19)
N(3)-Cu(1)-O(1)	96.14(14)	O(5A)-Cu(1)-N(3)	175.97(15)
N(3)-Cu(1)-O(7B)	93.40(14)	N(3)-Cu(1)-O(9)	86.09(17)
O(2C)-Cu(2)-O(3)	85.92(13)	O(2C)-Cu(2)-O(10)	174.58(13)
O(2C)-Cu(2)-O(11)	87.42(15)	O(3)-Cu(2)-O(10)	88.66(14)
O(3)-Cu(2)-O(11)	101.02(15)	O(10)-Cu(2)-O(11)	93.36(16)
O(2C)-Cu(2)-N(6)	99.04(14)	O(3)-Cu(2)-N(6)	170.93(15)
N(6)-Cu(2)-O(10)	86.37(15)	N(6)-Cu(2)-O(11)	86.86(15)

Symmetry codes: **1** A -x+1, y, -z+3/2; B -x+1/2, -y+1/2, -z+2**; 2** A x+1, -y+1/2, z-1/2; B -x,y+1/2,-z+1/2, C -x+1,-y+1,-z; **3** A -x+2, -y, -z+2; B x, -y+1/2, z+1/2; C -x+2, y-1/2, -z+3/2; **4** A -x+5/4, -y+1/4, z; B -x+5/4, y, -z+1/4; C x, -y+1/4, -z+1/4; **5** A -x+5/4, y, -z+1/4; B x, -y+1/4, -z+1/4; C -x+5/4, -y+1/4, z; **6** A -x+1, -y, -z; **7** A x+1, y+1, z; B x, y+1, z; C x-1, y, z.

Table S2. Hydrogen bonds for 1 (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1)-H(1W)···O(4)[a]	0.85(3)	1.95(3)	2.797(3)	171(3)
O(2)-H(2W)···O(4)[b]	0.79(3)	2.01(3)	2.790(3)	166(4)

Symmetry transformations used to generate equivalent atoms: a x, -y+1, z-1/2; b x, -y, z-1/2.

Table S3. Hydrogen bonds for 4 (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1)-H(1W)···O(2)	0.71(4)	2.13(4)	2.827(6)	168(5)
O(1)-H(1W)···O(5)[a]	0.71(4)	2.18(5)	2.87(2)	160(5)

Symmetry transformations used to generate equivalent atoms: a -x+3/4, -y-1/4, z.

Table S4. Hydrogen bonds for 4 (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1)-H(1W)···O(2)[a]	0.74(6)	2.10(6)	2.772(7)	151(6)
O(1)-H(1W)···O(3)[b]	0.74(6)	2.43(7)	3.14(3)	162(6)
O(1)-H(1W)···O(6)[b]	0.74(6)	2.05(7)	2.76(3)	163(6)

Symmetry transformations used to generate equivalent atoms: a x-1/2, y-1/2, z; b -x+5/4, -y+1/4, z.

Table S5. Hydrogen bonds for 7 (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(9)-H(1W)···O(13)[a]	0.78(4)	1.93(6)	2.630(9)	150(8)
O(9)-H(2W)···O(6)[b]	0.78(5)	2.25(7)	2.742(6)	121(7)
O(9)-H(2W)···O(13)	0.78(5)	2.33(5)	3.053(9)	155(8)
O(10)-H(3W)···O(4)	0.85(4)	1.71(4)	2.547(5)	168(6)
O(10)-H(4W)···O(7)[c]	0.90(4)	1.83(5)	2.714(5)	165(7)
O(11)-H(6W)···O(11)[d]	0.80(4)	2.00(5)	2.784(9)	168(9)

Symmetry transformations used to generate equivalent atoms: a -x+2, -y+2, -z+2; b x+1, y+1, z; c x, y+1, z; d -x, -y+1, -z+1.

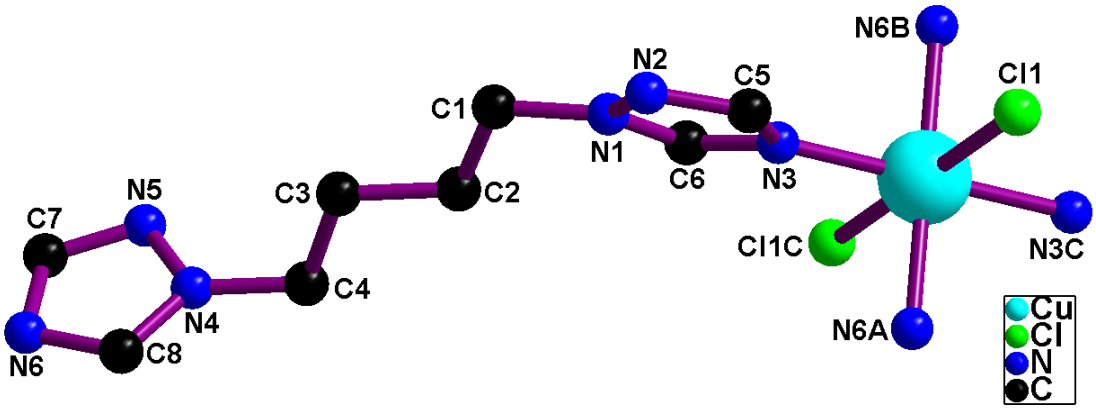

Fig. S1 The coordination environment of Cu(II) atom of **2**.

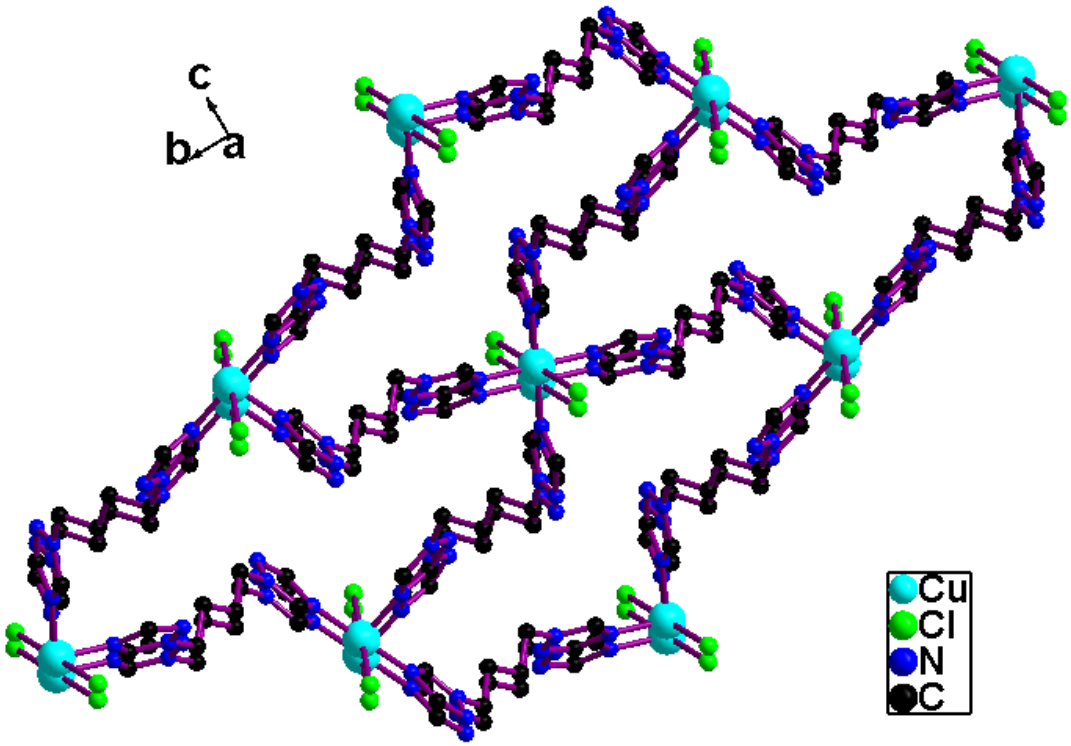

Fig. S2 The parallel stacking of two 2D (4,4) networks of **2**.

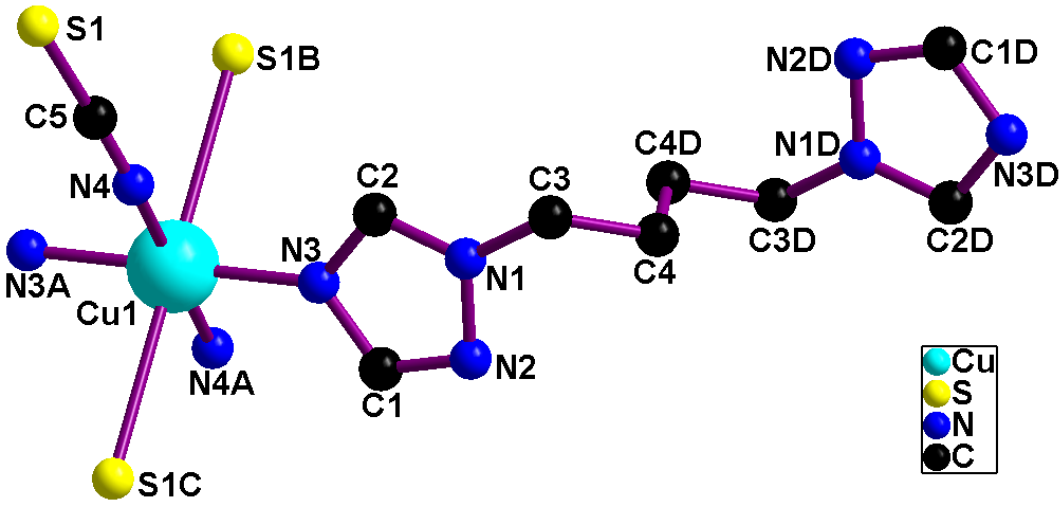

Fig. S3 The coordination environment of the Cu(II) atom of **3**.

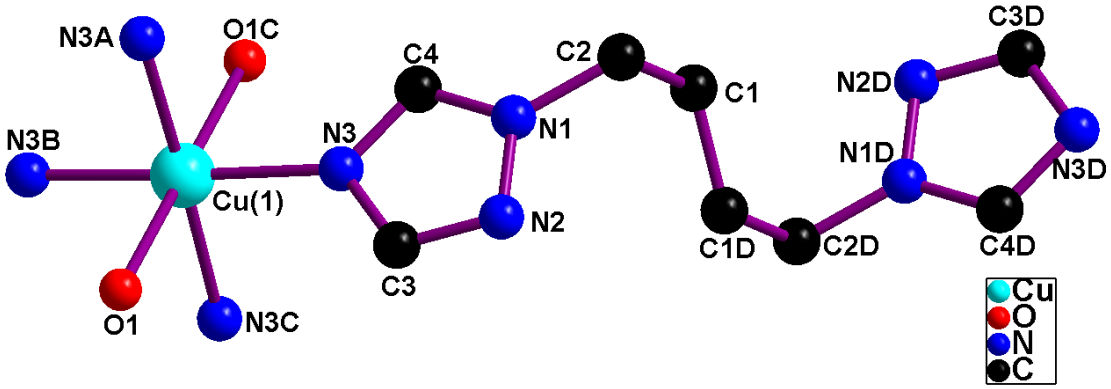

Fig. S4 The coordination environment of the Cu(II) atom of **4**. CubtbClO4

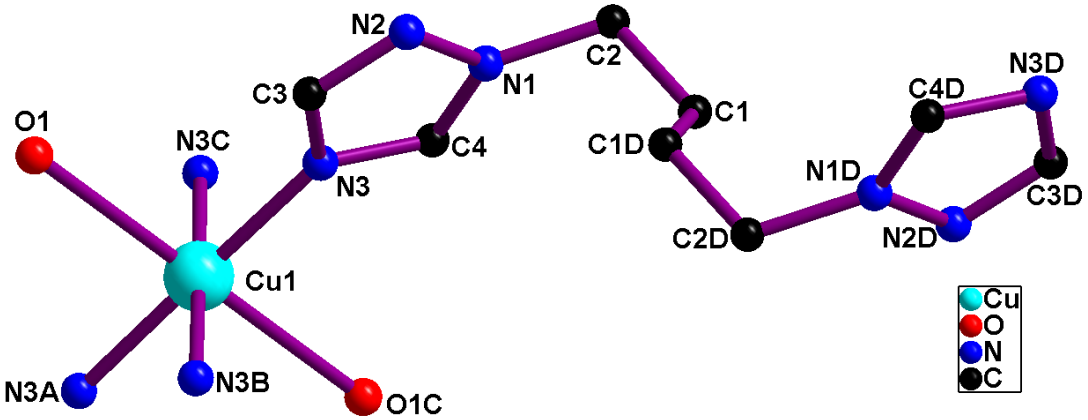

Fig. S5 The coordination environment of the Cu(II) atom of **5**.

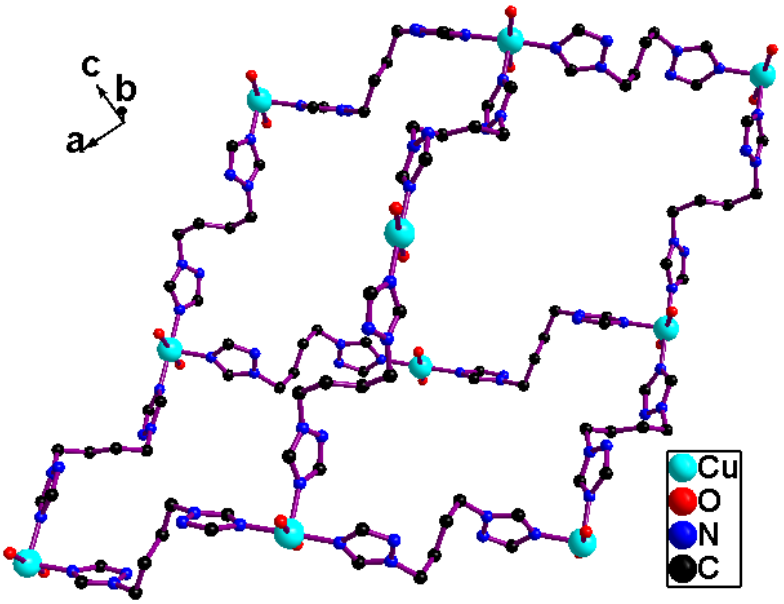

Fig. S6 Single adamantanoid cage of **4** and **5**.

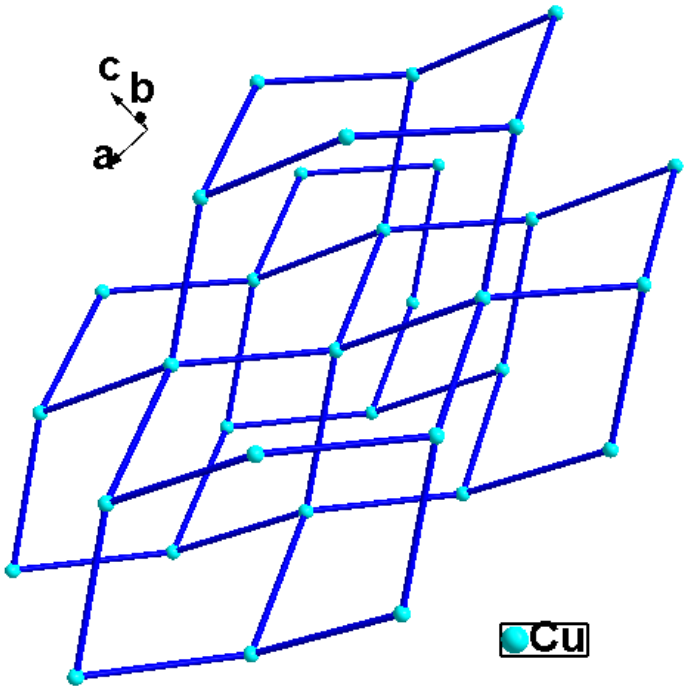

Fig. S7 Schematic depiction of a single diamondoid network of **4** and **5**.

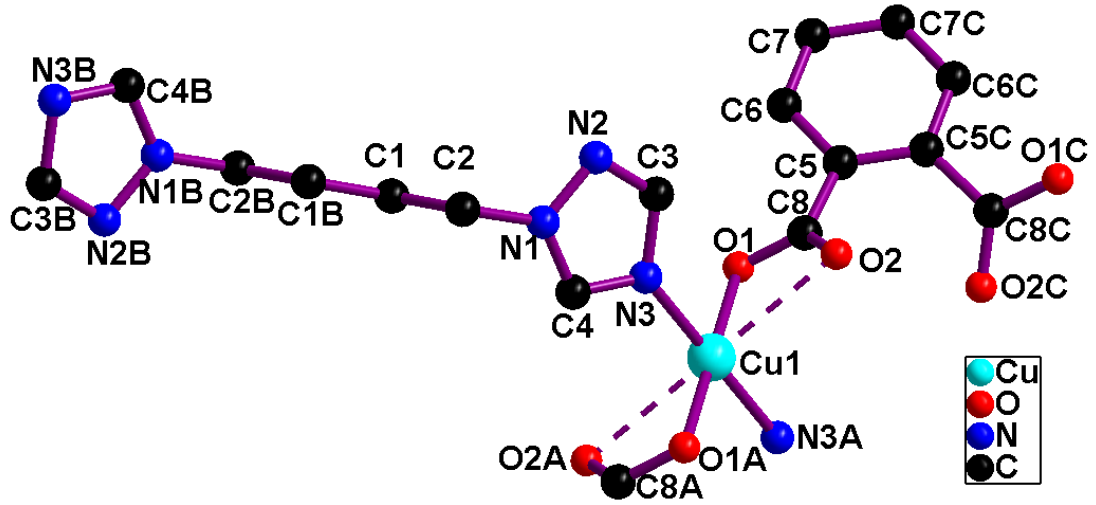

Fig. S8 The coordination environment of Cu(II) atom of **6**.

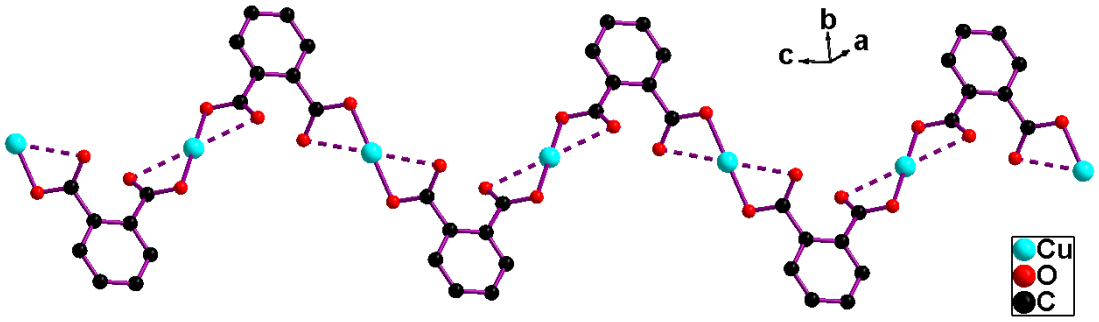

Fig. S9 A 1D $[Cu(bdc)]_n$ chain of **6**.

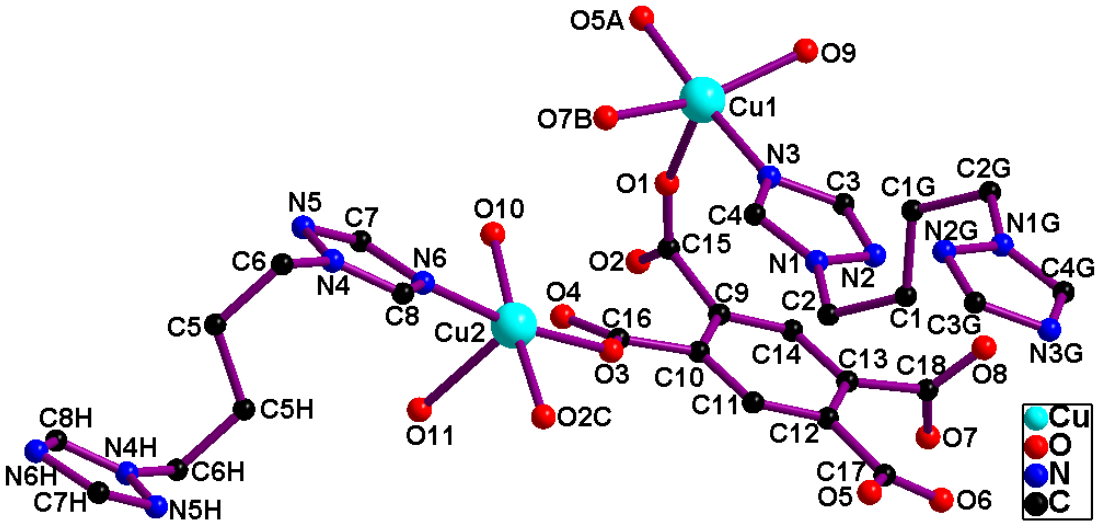

Fig. S10 The coordination environment of two Cu(II) atoms of **7**.

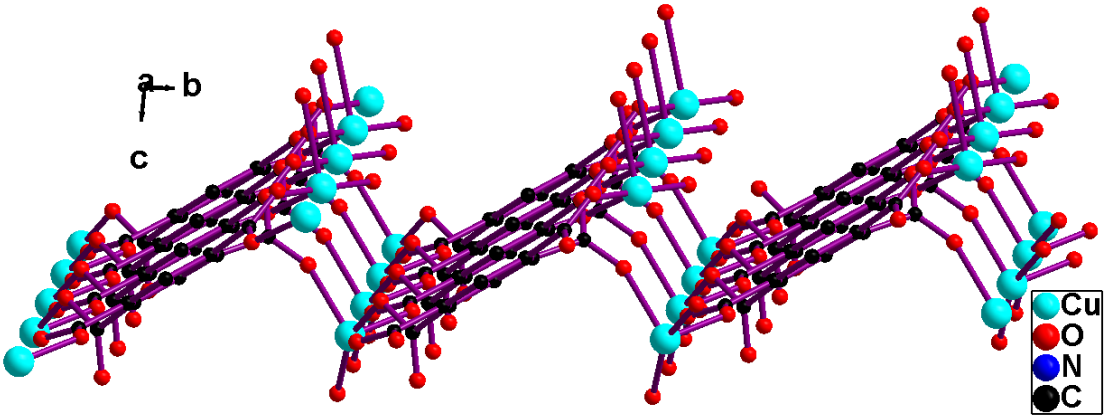

Fig. S11 Viewing a 2D $[Cu_2(btec)(H_2O)_3]_n$ network of **7** along the *a* direction.

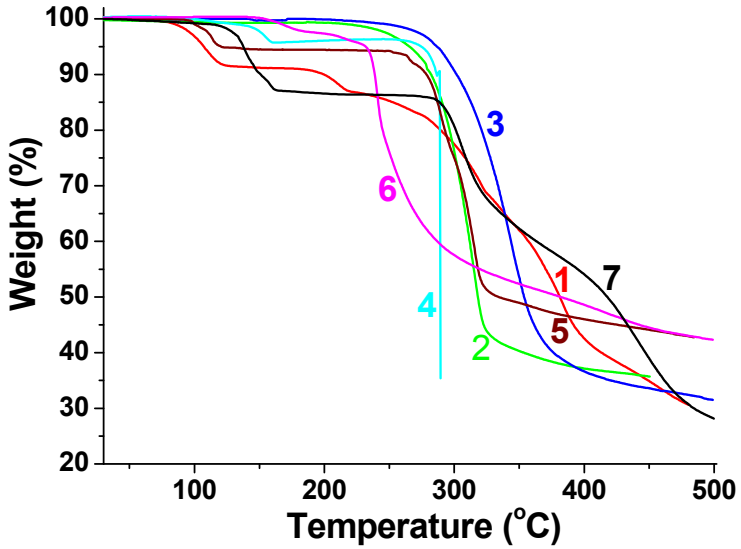

Fig. S12 TG curves of complexes **1-7**.