

Chloranilate bridged dinuclear copper(II) complexes: *Syn-anti* geometry tuned by steric factor and supramolecular interactions

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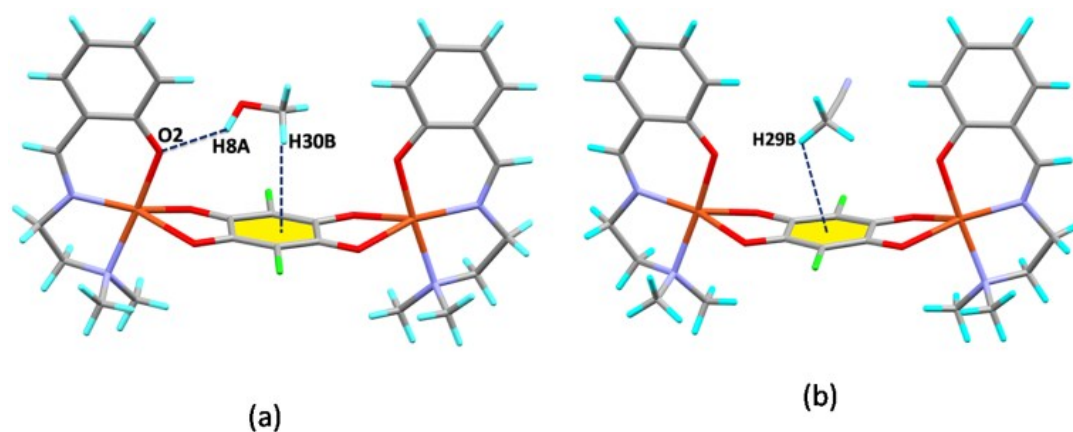


Figure S1. Stabilisation of *syn* form by C–H... π and hydrogen bonding interactions in **1** (a) and **1A** (b).

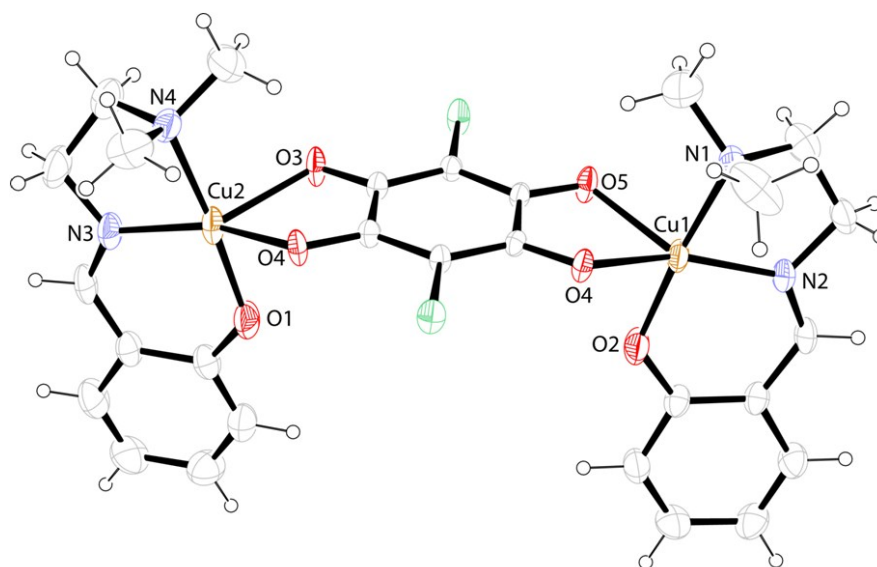


Fig. S2: ORTEP diagram of complex **1A** with 30% ellipsoid probability. CH₃CN has been removed for clarity.

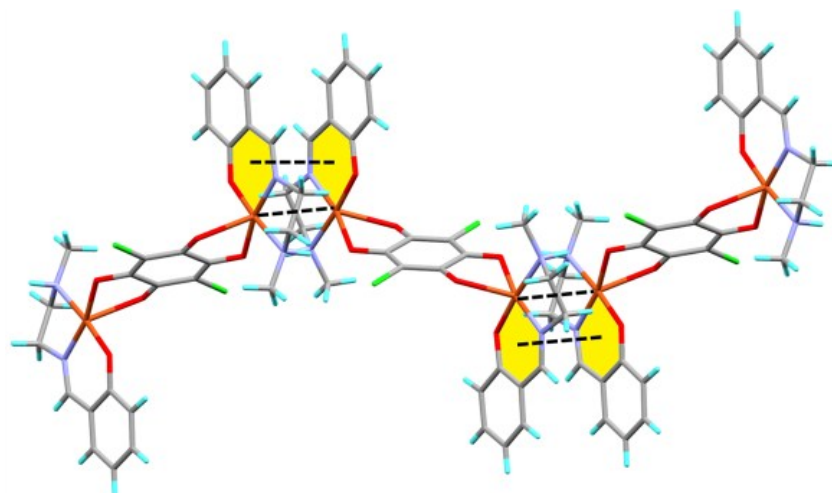


Figure S3. Formation of 1D supramolecular framework of complex **2**.

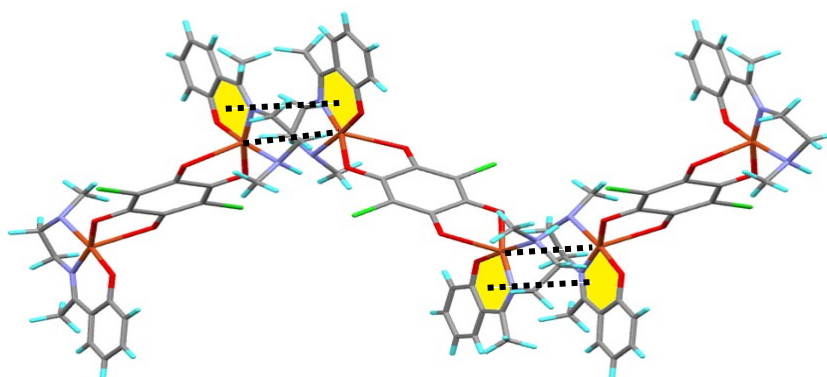


Fig. S4:Formation of 1D supramolecular framework of complex **3** by chelate ring•••chelate ring π -stacking and cuprophilic interactions

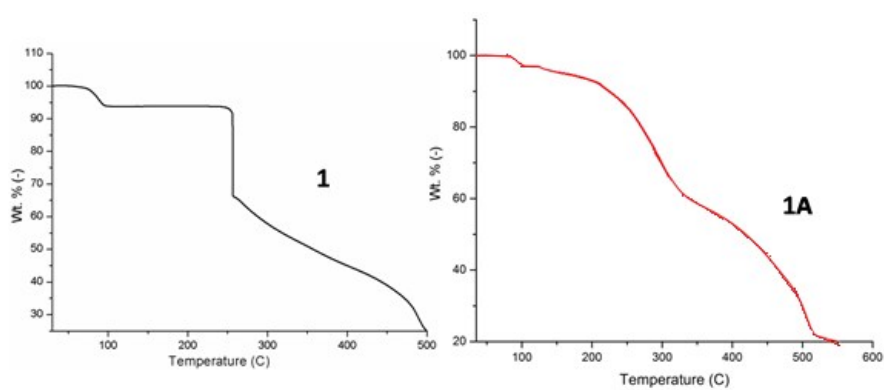


Fig. S5:TG data of complexes **1** and **1A**.

Table S1: Selected bond lengths(Å) and angles(°) of complexes **1**, **1A**, **2** and **3**.

Bond distances(Å)							
1		1A		2		3	
Cu(1)-O(1)	1.882(6)	Cu(1)-O(2)	1.906(4)	Cu(1)-O(1)	1.908(5)	Cu(1)-O(4)	2.273(3)
Cu(1)-O(3)	2.121(5)	Cu(1)-O(5)	2.113(4)	Cu(1)-O(2)	2.053(4)	Cu(1)-O(5)	2.033(4)
Cu(1)-O(4)	2.150(5)	Cu(1)-O(6)	2.147(4)	Cu(1)-N(1)	2.026(5)	Cu(1)-O(6)	1.861(4)
Cu(1)-N(1)	1.918(5)	Cu(1)-N(1)	2.060(5)	Cu(1)-N(2)	1.929(6)	Cu(1)-N(1)	1.939(5)
Cu(1)-N(2)	2.045(6)	Cu(1)-N(2)	1.925(5)	Cu(1)-O(3) ^a	2.282(4)	Cu(1)-N(2)	2.013(5)
Cu(2)-O(2)	1.889(5)	Cu(2)-O(1)	1.920(5)			Cu(2)-O(1)	2.031(4)
Cu(2)-O(5)	2.102(5)	Cu(2)-O(3)	2.088(4)			Cu(2)-O(2)	2.256(3)
Cu(2)-O(6)	2.148(5)	Cu(2)-O(4)	2.155(4)			Cu(2)-O(3)	1.855(4)
Cu(2)-N(3)	2.071(5)	Cu(2)-N(3)	1.930(5)			Cu(2)-N(3)	2.003(5)
Cu(2)-N(4)	1.891(6)	Cu(2)-N(4)	2.060(5)			Cu(2)-N(4)	1.948(5)
Bond angles(°)							
1		1A		2		3	
O(1)-Cu(1)-O(3)	89.0(2)	O(2)-Cu(1)-O(5)	88.6(2)	O(1)-Cu(1)-O(2)	88.0(2)	O(4)-Cu(1)-O(5)	75.6(1)
O(1)-Cu(1)-O(4)	88.8(2)	O(2)-Cu(1)-O(6)	90.9(2)	O(1)-Cu(1)-N(1)	174.0(2)	O(4)-Cu(1)-O(6)	91.1(2)
O(1)-Cu(1)-N(1)	94.5(2)	O(2)-Cu(1)-N(1)	174.1(2)	O(1)-Cu(1)-N(2)	92.3(2)	O(4)-Cu(1)-N(1)	115.5(2)
O(1)-Cu(1)-N(2)	175.0(2)	O(2)-Cu(1)-N(2)	92.9(2)	O(1)-Cu(1)-O(3) ^a	88.3(2)	O(4)-Cu(1)-N(2)	95.4(2)
O(3)-Cu(1)-O(4)	76.4(2)	O(5)-Cu(1)-O(6)	76.7(1)	O(2)-Cu(1)-N(1)	92.6(2)	O(5)-Cu(1)-O(6)	86.9(2)
O(3)-Cu(1)-N(1)	136.1(2)	O(5)-Cu(1)-N(1)	91.6(2)	O(2)-Cu(1)-N(2)	165.2(2)	O(5)-Cu(1)-N(1)	168.9(2)
O(3)-Cu(1)-N(2)	95.9(2)	O(5)-Cu(1)-N(2)	152.3(2)	O(2)-Cu(1)-O(3) ^a	74.9(1)	O(5)-Cu(1)-N(2)	91.5(2)
O(4)-Cu(1)-N(1)	147.3(2)	O(6)-Cu(1)-N(1)	94.9(2)	N(1)-Cu(1)-N(2)	85.6(2)	O(6)-Cu(1)-N(1)	93.1(2)
O(4)-Cu(1)-N(2)	91.6(2)	O(6)-Cu(1)-N(2)	130.8(2)	N(1)-Cu(1)-O(3) ^a	97.6(2)	O(6)-Cu(1)-N(2)	172.7(2)
N(1)-Cu(1)-N(2)	82.6(2)	O(5)-Cu(1)-N(2)	152.3(2)	N(2)-Cu(1)-O(3) ^a	119.9(2)	N(1)-Cu(1)-N(2)	87.2(2)
O(2)-Cu(2)-O(5)	88.8(2)	N(1)-Cu(1)-N(2)	84.2(2)			O(1)-Cu(2)-O(2)	75.9(1)
O(2)-Cu(2)-O(6)	87.9(2)	O(1)-Cu(2)-O(3)	88.7(2)			O(1)-Cu(2)-O(3)	88.7(2)
O(2)-Cu(2)-N(3)	175.0(2)	O(1)-Cu(2)-O(4)	90.0(2)			O(1)-Cu(2)-N(3)	89.3(2)
O(2)-Cu(2)-N(4)	97.5(2)	O(1)-Cu(2)-N(3)	92.9(2)			O(1)-Cu(2)-N(4)	165.5(2)
O(5)-Cu(2)-O(6)	76.7(2)	O(1)-Cu(2)-N(4)	175.0(2)			O(2)-Cu(2)-O(3)	91.0(2)
O(5)-Cu(2)-N(3)	96.1(2)	O(3)-Cu(2)-O(4)	77.0(1)			O(2)-Cu(2)-N(3)	94.9(2)
O(5)-Cu(2)-N(4)	136.7(2)	O(3)-Cu(2)-N(3)	153.3(2)			O(2)-Cu(2)-N(4)	118.4(2)
O(6)-Cu(2)-N(3)	92.6(2)	O(3)-Cu(2)-N(4)	91.7(2)			O(3)-Cu(2)-N(3)	173.6(2)
O(6)-Cu(2)-N(4)	145.9(2)	O(4)-Cu(2)-N(3)	129.6(2)			O(3)-Cu(2)-N(4)	92.7(2)
N(3)-Cu(2)-N(4)	79.3(2)	O(4)-Cu(2)-N(4)	95.0(2)			N(3)-Cu(2)-N(4)	86.9(2)
		N(3)-Cu(2)-N(4)	84.5(2)				

^a = 1/2-x,3/2-y,1-z (for complex **2**)