

Supporting material

Open and Closed Copper Chain Coordination Polymers with Alternating Ferromagnetic and Antiferromagnetic Interaction

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Table S1 selected bond length and angles of **1**

Cu(1)-O(1)	1.931(3)	Cu(1)-O(5)	2.173(3)
Cu(1)-O(7)	1.954(4)	Cu(2)-O(9)	1.947(3)
Cu(1)-O(8)	1.965(3)	Cu(2)-O(6)	1.949(3)
Cu(1)-N(1)	2.036(4)	O(1)-Cu(1)-O(5)	97.00(15)
O(1)-Cu(1)-O(8)	154.97(15)	O(7)-Cu(1)-O(5)	98.91(15)
O(7)-Cu(1)-O(8)	92.37(15)	O(8)-Cu(1)-O(5)	106.63(14)
O(1)-Cu(1)-N(1)	90.01(14)	N(1)-Cu(1)-O(5)	79.77(13)
O(7)-Cu(1)-N(1)	177.69(14)	O(9)-Cu(2)-O(6)	85.11(13)
O(1)-Cu(1)-O(7)	92.04(15)	O(9)-Cu(2)-O(6)	94.89(13)
O(8)-Cu(1)-N(1)	86.22(14)		

Symmetry transformation used to generate equivalent atoms: a -x,-y+1,-z+1, b -x+1,-y+1,-z+1

Table S2 Selected bond length and angles for **2**

Cu(4)-O(24)	1.931(5)	Cu(3)-O(21)	1.948(7)
Cu(4)-O(13)	1.975(6)	Cu(3)-O(22)	1.952(6)
Cu(4)-O(9)	1.983(6)	Cu(3)-O(7)	1.956(6)
Cu(4)-N(2)	2.000(6)	Cu(3)-O(12)	1.961(6)
Cu(4)-O(11)	2.147(6)	Cu(3)-O(23)	2.407(8)
Cu(1)-O(15)	1.923(5)	Cu(2)-O(20)	1.914(6)
Cu(1)-O(1)	1.939(5)	Cu(2)-O(5)	1.940(6)
Cu(1)-O(18)	1.996(6)	Cu(2)-O(2)	1.994(5)
Cu(1)-O(19)	2.009(6)	Cu(2)-N(1)	2.017(6)
Cu(1)-O(17)	2.220(6)	Cu(2)-O(3)	2.236(5)
O(15)-Cu(1)-O(1)	177.9(3)	O(7)-Cu(3)-O(23)	92.9(3)
O(15)-Cu(1)-O(18)	86.7(3)	O(12)-Cu(3)-O(23)	99.9(2)
O(1)-Cu(1)-O(18)	91.9(3)	O(21)-Cu(3)-O(22)	166.7(4)
O(15)-Cu(1)-O(19)	95.1(3)	O(21)-Cu(3)-O(7)	88.0(3)
O(1)-Cu(1)-O(19)	86.6(3)	O(22)-Cu(3)-O(7)	94.4(3)
O(18)-Cu(1)-O(19)	164.0(3)	O(21)-Cu(3)-O(12)	89.2(3)
O(15)-Cu(1)-O(17)	92.2(3)	O(22)-Cu(3)-O(12)	85.5(3)
O(1)-Cu(1)-O(17)	86.4(2)	O(7)-Cu(3)-O(12)	167.1(3)
O(18)-Cu(1)-O(17)	100.4(3)	O(21)-Cu(3)-O(23)	94.9(3)

O(19)-Cu(1)-O(17)	95.4(3)	O(22)-Cu(3)-O(23)	98.0(3)
O(20)-Cu(2)-O(2)	91.8(3)	O(24)-Cu(4)-O(13)	93.6(2)
O(5)-Cu(2)-O(2)	155.2(2)	O(24)-Cu(4)-O(9)	95.2(2)
O(20)-Cu(2)-N(1)	171.1(3)	O(13)-Cu(4)-O(9)	148.2(2)
O(5)-Cu(2)-N(1)	84.9(2)	O(24)-Cu(4)-N(2)	174.3(2)
O(20)-Cu(2)-O(5)	91.9(3)	O(13)-Cu(4)-N(2)	84.2(2)
O(2)-Cu(2)-N(1)	87.7(2)	O(9)-Cu(4)-N(2)	89.4(2)
O(20)-Cu(2)-O(3)	110.2(3)	O(24)-Cu(4)-O(11)	95.8(2)
O(5)-Cu(2)-O(3)	114.0(2)	O(13)-Cu(4)-O(11)	115.8(3)
O(2)-Cu(2)-O(3)	87.6(2)	O(9)-Cu(4)-O(11)	93.6(2)
N(1)-Cu(2)-O(3)	78.6(2)	N(2)-Cu(4)-O(11)	80.5(2)

Table S3 H-bond data in **2**

D-H...A	<DHA	D(D...A)
O22-H22...O4a	168.4(5)	2.74(2)
O24-H24...O3b	147.6(0)	2.75(9)
O19-H19...O8c	137.1(5)	2.74(2)
O17-H17...O28c	121.4(4)	2.86(4)
O21-H21...O28d	153.0(9)	2.67(4)
O20-H20...O4e	151.1(7)	2.64(6)
O23-H23...O16b	151.4(7)	3.07(9)
O18-H18A...O10f	140.0(9)	2.76(0)
O21-H25...O27g	163.1(1)	3.09(3)
O22-H26...O8	160.3(2)	3.15(2)
O22-H26...O7	112.8(9)	2.86(6)
O22-H26...O19a	127.8(5)	3.08(1)
O24-H27...O26d	149.1(5)	2.60(3)
O19-H50...O10h	128.4(9)	2.79(1)
O23-H52...O20b	119.7(9)	2.73(0)
O20-H53...O23i	176.8(7)	2.73(0)
O25-H54...O14f	147.3(4)	2.74(3)
O25-H55...O16b	172.5(3)	2.87(7)
O28-H56...O9j	123.9(7)	2.89(9)
O28-H57...O17a	112.9(3)	2.86(4)
O26-H59...O25j	130.9(2)	2.81(5)
O28-H57...O17a	112.9(3)	2.86(4)
O26-H59...O25j	130.9(2)	2.81(5)
O26-H59...O12k	126.7(9)	3.09(3)
O26-H58...O24j	113.4(9)	2.60(3)

Symmetry transformation used to generate equivalent atoms: a -x, y+1/2, -z+1; b -x+1, y+1/2, -z+1; c -x, y-1/2, -z+1; d x, y, z-1; e x+1, y, z; f -x+1, y-1/2, -z; g -x+1, y+1/2, -z; h -x, y-1/2, -z; i -x+1, y-1/2, -z+1; j x, y, z+1; k x+1, y, z+1.

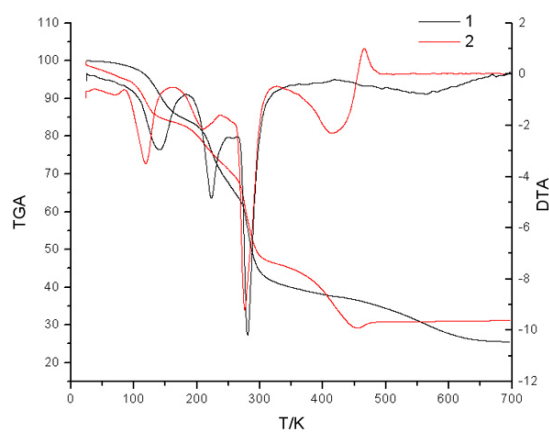


Figure S1 TGA and DTA analysis of **1** and **2**

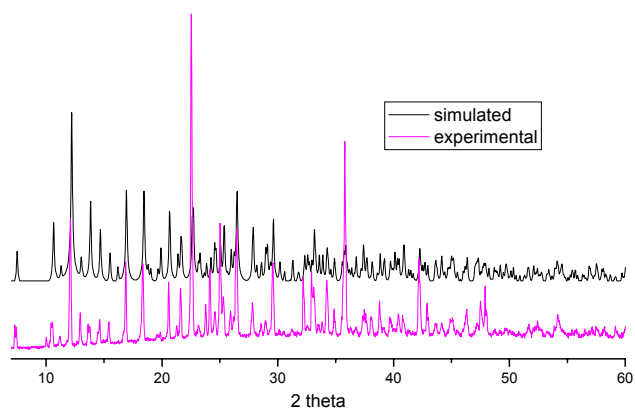


Figure S2 Experimental and simulated (from single crystal diffraction data of **1**)
PXRD patterns for **1**

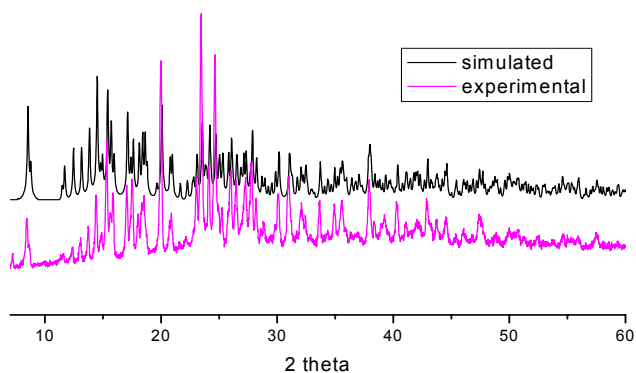


Figure S3 Experimental and simulated (from single crystal diffraction data of **2**)
PXRD patterns for **2**