Electronic Supplementary Material for CrystEngComm

Supporting information

The Nanoscale Drum-Gong-Cymbals-Like Mixed-Valence $Cu^{II}Cu^{I}_{3}$ Cluster Polymer and Magnetism Study

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1. Perspective View for compound 1

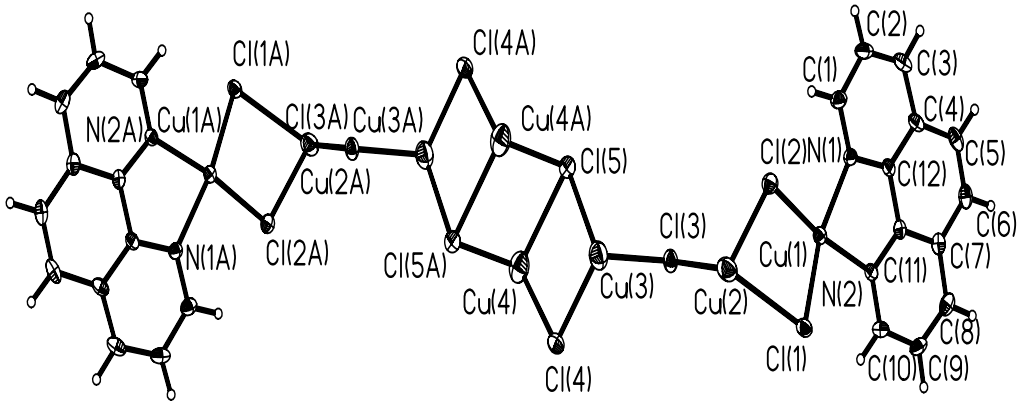

Fig. S1. ORTEP drawing of structural unit for compound 1

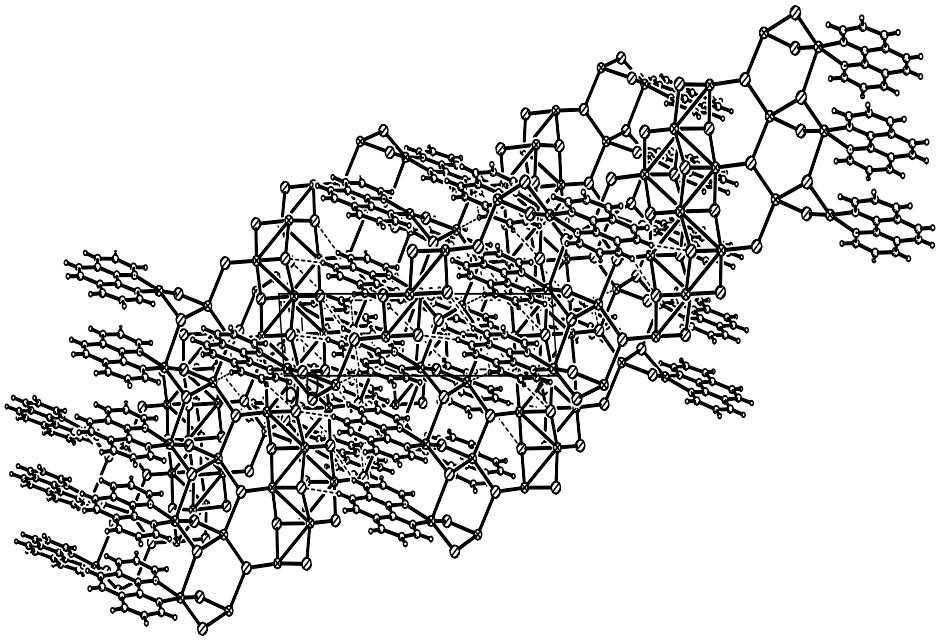

Fig. S2. The packing diagram of the complex 1 viewed along *b* axis

2. Crystallographic data for the compound 1

Table S1. Crystal data and structure refinement for compound **1**

Empirical formula	$C_{12}H_8Cl_5Cu_4N_2$
Formula weight	611.61
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 3.7700(8) Å α = 90 ° b = 25.660(5) Å β = 95.23(3)°. c = 16.430(3) Å γ = 90°.
Volume	1582.8(5) $Å^3$
Z, Calculated density	4, 2.567 Mg/m^3
Absorption coefficient	6.139 mm^{-1}
F(000)	1180
Theta range for data collection	1.48 to 25.00°.
Limiting indices	$-4 \le h \le 3, -29 \le k \le 30, -19 \le l \le 18$
Reflections collected / unique	8378 / 2809 [$R_{(int)}$ =0.0509]
Completeness to theta	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2809 / 0 / 209
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R_1 =0.0435, wR_2 =0.1006
R indices (all data)	R_1 = 0.0673, wR_2 =0.1130
Largest diff. peak and hole	0.773 and -0.811e. $Å^{-3}$

3. Table of bond lengths and angles for compound 1

Table S2. Bond lengths [Å] and angles [deg] for compound **1**

Cu(1)-N(2)	2.000(5)	N(2)-Cu(1)-N(1)	81.44(18)	Cl(5)#3-Cu(4)-Cl(4)#1	121.93(8)
Cu(1)-N(1)	2.025(5)	N(2)-Cu(1)-Cl(2)	169.57(14)	Cl(5)#3-Cu(4)-Cl(4)	116.47(7)
Cu(1)-Cl(2)	2.2572(16)	N(1)-Cu(1)-Cl(2)	92.50(14)	Cl(4)#1-Cu(4)-Cl(4)	111.40(8)
Cu(1)-Cl(1)	2.2650(16)	N(2)-Cu(1)-Cl(1)	92.10(13)	Cl(5)#3-Cu(4)-Cl(5)	101.33(6)
Cu(1)-Cl(1)#1	2.7564(19)	N(1)-Cu(1)-Cl(1)	162.76(15)	Cl(4)#1-Cu(4)-Cl(5)	98.92(7)
Cu(2)-Cl(3)#2	2.2149(18)	Cl(2)-Cu(1)-Cl(1)	91.30(6)	Cl(4)-Cu(4)-Cl(5)	101.96(7)
Cu(2)-Cl(2)	2.2477(18)	N(2)-Cu(1)-Cl(1)#1	90.45(14)	Cl(5)#3-Cu(4)-Cu(3)	120.63(6)
Cu(2)-Cl(3)	2.409(2)	N(1)-Cu(1)-Cl(1)#1	99.18(15)	Cl(4)#1-Cu(4)-Cu(3)	113.94(6)
Cu(2)-Cl(1)	2.6588(18)	Cl(2)-Cu(1)-Cl(1)#1	98.92(6)	Cl(4)-Cu(4)-Cu(3)	52.38(5)
Cu(3)-Cl(3)	2.2640(18)	Cl(1)-Cu(1)-Cl(1)#1	96.83(6)	Cl(5)-Cu(4)-Cu(3)	49.59(5)
Cu(3)-Cl(4)	2.3626(18)	Cl(3)#2-Cu(2)-Cl(2)	144.90(8)	Cl(5)#3-Cu(4)-Cu(3)#1	123.32(6)
Cu(3)-Cl(5)	2.372(2)	Cl(3)#2-Cu(2)-Cl(3)	109.18(8)	Cl(4)#1-Cu(4)-Cu(3)#1	50.50(5)
Cu(3)-Cl(5)#2	2.3774(19)	Cl(2)-Cu(2)-Cl(3)	101.81(7)	Cl(4)-Cu(4)-Cu(3)#1	116.32(6)
Cu(3)-Cu(4)	2.9117(18)	Cl(3)#2-Cu(2)-Cl(1)	97.96(6)	Cl(5)-Cu(4)-Cu(3)#1	48.42(4)
Cu(3)-Cu(4)#2	3.0291(17)	Cl(2)-Cu(2)-Cl(1)	82.00(6)	Cu(3)-Cu(4)-Cu(3)#1	78.75(4)
Cu(4)-Cl(5)#3	2.2468(18)	Cl(3)-Cu(2)-Cl(1)	116.67(6)	Cu(1)-Cl(1)-Cu(2)	84.16(5)
Cu(4)-Cl(4)#1	2.2723(19)	Cl(3)-Cu(3)-Cl(4)	114.94(7)	Cu(1)-Cl(1)-Cu(1)#2	96.83(6)
Cu(4)-Cl(4)	2.291(2)	Cl(3)-Cu(3)-Cl(5)	108.24(7)	Cu(2)-Cl(1)-Cu(1)#2	101.38(6)
Cu(4)-Cl(5)	2.730(2)	Cl(4)-Cu(3)-Cl(5)	111.40(7)	Cu(2)-Cl(2)-Cu(1)	94.67(6)
Cu(4)-Cu(3)#1	3.0291(17)	Cl(3)-Cu(3)-Cl(5)#2	109.61(8)	Cu(2)#1-Cl(3)-Cu(3)	119.37(8)
Cl(1)-Cu(1)#2	2.7564(19)	Cl(4)-Cu(3)-Cl(5)#2	107.11(7)	Cu(2)#1-Cl(3)-Cu(2)	109.18(8)
Cl(3)-Cu(2)#1	2.2149(18)	Cl(5)-Cu(3)-Cl(5)#2	105.09(7)	Cu(3)-Cl(3)-Cu(2)	115.34(7)
Cl(4)-Cu(4)#2	2.2723(19)	Cl(3)-Cu(3)-Cu(4)	130.65(6)	Cu(4)#2-Cl(4)-Cu(4)	111.40(8)
Cl(5)-Cu(4)#3	2.2468(18)	Cl(4)-Cu(3)-Cu(4)	50.18(5)	Cu(4)#2-Cl(4)-Cu(3)	81.59(7)
Cl(5)-Cu(3)#1	2.3774(19)	Cl(5)-Cu(3)-Cu(4)	61.22(5)	Cu(4)-Cl(4)-Cu(3)	77.44(7)
		Cl(5)#2-Cu(3)-Cu(4)	119.73(6)	Cu(4)#3-Cl(5)-Cu(3)	113.53(7)
		Cl(3)-Cu(3)-Cu(4)#2	130.13(6)	Cu(4)#3-Cl(5)-Cu(3)#1	118.31(8)
		Cl(4)-Cu(3)-Cu(4)#2	47.91(5)	Cu(3)-Cl(5)-Cu(3)#1	105.09(7)
		Cl(5)-Cu(3)-Cu(4)#2	121.63(6)	Cu(4)#3-Cl(5)-Cu(4)	78.67(6)
		Cl(5)#2-Cu(3)-Cu(4)#2	59.20(5)	Cu(3)-Cl(5)-Cu(4)	69.20(6)
		Cu(4)-Cu(3)-Cu(4)#2	78.75(4)	Cu(3)#1-Cl(5)-Cu(4)	72.38(6)

#1 *x-1, y, z* #2 *x+1, y, z* #3 *-x-2, -y, -z-1*

4. Table of *π*-*π* Interactions and C-*π* Interactions

Table S3. Geometrical Parameters of Hydrogen Bonds (Å, deg) for **1**

D-H···A	Symmetry code	D - H	D···A	D - H...A
C(1)-H(1A)…Cl(2)	*Intra*	0.9300	3.2134	118.71
C(5)-H(5A) …Cl(4)	*x, y, 1+z*	0.9300	3.6971	163.42
C(10)-H(10A)…Cl(1)	*Intra*	0.9300	3.2320	114.48

5. Table of *π*-*π* Interactions and C-H···*π* Interactions

Table S4. *π*-*π* Interactions in complex 1

ring(*i*)→ring(*j*)/C	Symmetry code	distance between the *(i,j)* ring centroids(Å)	dihedral angle (*i,j*) (°)	distance of centroid(*i*) from ring (*j*) (Å)
Cg(1) → Cg(1)	*1-x, -y, -1-z*	3.957	0.03	3.951
Cg(1) → Cg(2)	*1-x, -y, -1-z*	3.422	65.67	2.820
Cg(1) → Cg(3)	*-x, -y, -1-z*	3.422	65.67	2.820
Cg(1) →Cg(4)	*1+x, y, z/ 1-x, -y, -1-z*	3.349	59.34	2.805
Cg(2) →Cg(2)	*1-x, -y, -1-z*	3.857	0.03	3.834
Cg(2) → Cg(3)	*2+x, y, z*	3.770	0.03	2.028
Cg(2) → Cg(4)	*-x, -y, -1-z*	3.260	54.99	2.841
Cg(3) → Cg(3)	*-1-x, -y, -1-z*	3.857	0.04	3.834
Cg(3) → Cg(4)	*-1-x, -y, -1-z*	3.260	54.99	2.841
Cg(4) → Cg(4)	*-1-x, -y, -1-z /1-x, -y, -1-z*	3.770	3.4315	3.765
Cg(5) →Cg(6)	*1+x, y, z*	3.494	5.4512	3.410
Cg(5) → Cg(7)	*1+x, y, z*	3.876	5.4878	3.411
Cg(8) → Cg(7)	*1+x, y, z*	3.560	5.4878	3.454
Cg(5) → Cu(1)	*-1+x, y, z*	3.651	22.84	3.365
Cg(6) → Cu(1)	*-1+x, y, z*	3.841	30.51	3.309

Cg(1):Cu(3)-Cl(4)-Cu(4)-Cl(5); Cg(2): Cu(3)-Cl(4)-Cu(4)b-Cl(5)b; Cg(3): Cu(4)-Cl(5)- Cu(3)a-Cl(4)a; Cg(4): Cu(4)-Cl(5)-Cu(4)c-Cl(5)c; Cg(5): Cu(1)-N(1)-C(12)-C(11)-N(2); Cg(6): N(1)-C(1)-C(2)-C(3)-C(4)-C(12); Cg(7): N(2)-C(10)-C(9)-C(8)-C(7)-C(11); Cg(8): C(4)-C(5)- C(6)-C(7)-C(11)-C(12).

6. Magnetic Properties of compound 1

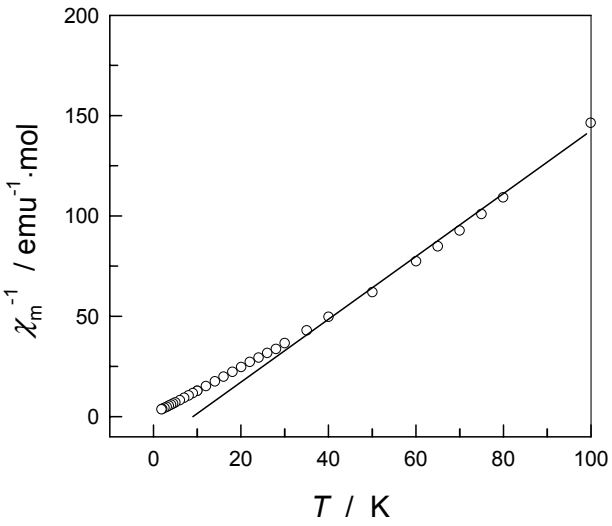

Figure S3. Temperature dependence of the X_M^{-1} of 1

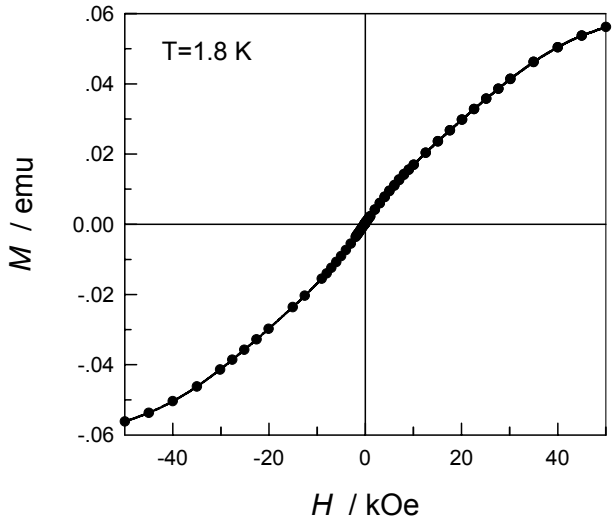

Figure S4. Field-dependent magnetization of **1** at 1.8K.