Supporting Information

Switchable dielectric phase transition behaviors in two organic-inorganic copper(II) halides with distinct coordination geometries†

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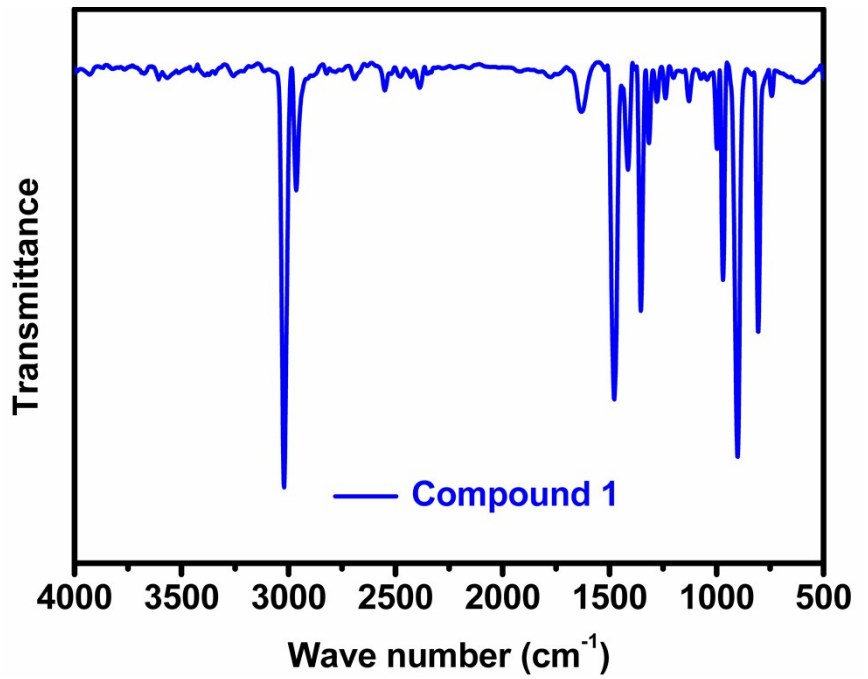

Fig. S1 Infrared (IR) spectrum of solid **1** in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at room temperature.

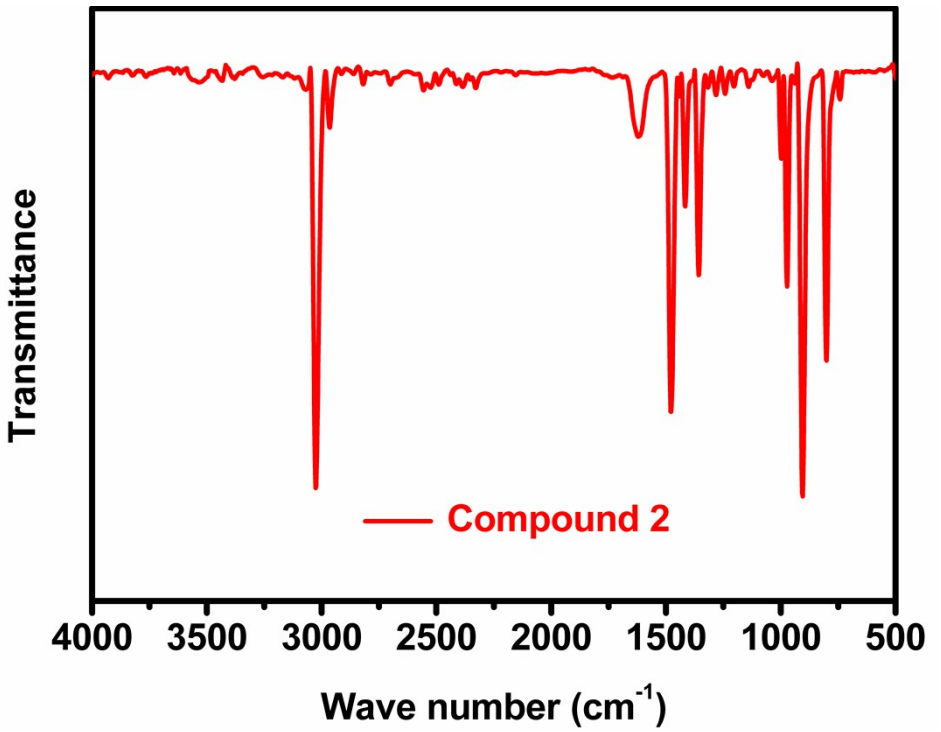

Fig. S2 Infrared (IR) spectrum of solid **2** in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at room temperature.

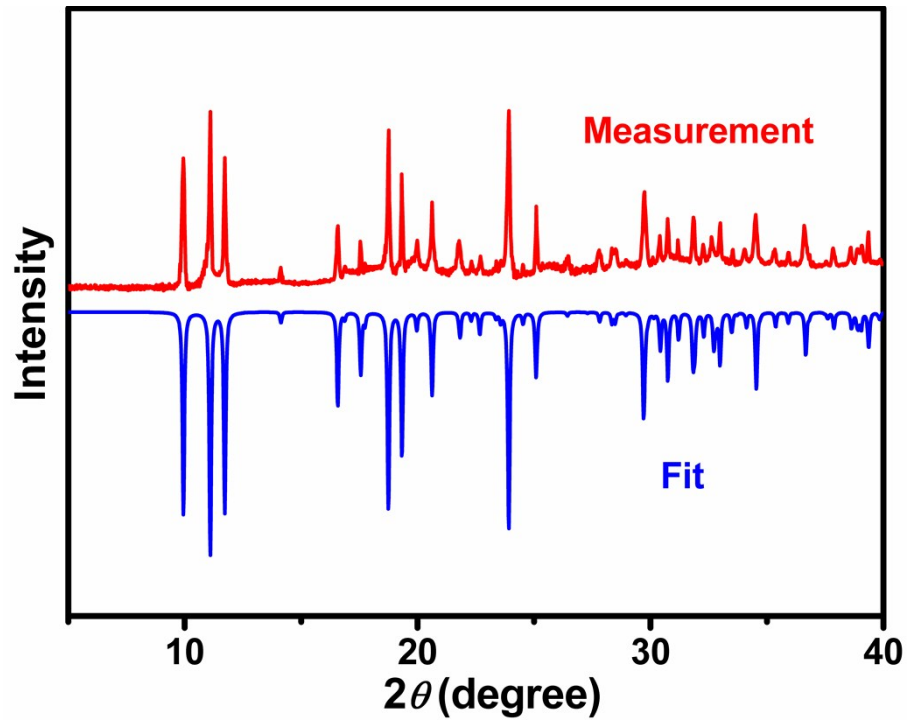

Fig. S3 Experimental powder diffraction (XRPD) patterns matching well with the simulated ones in terms of the crystal structures in **2** at 293 K.

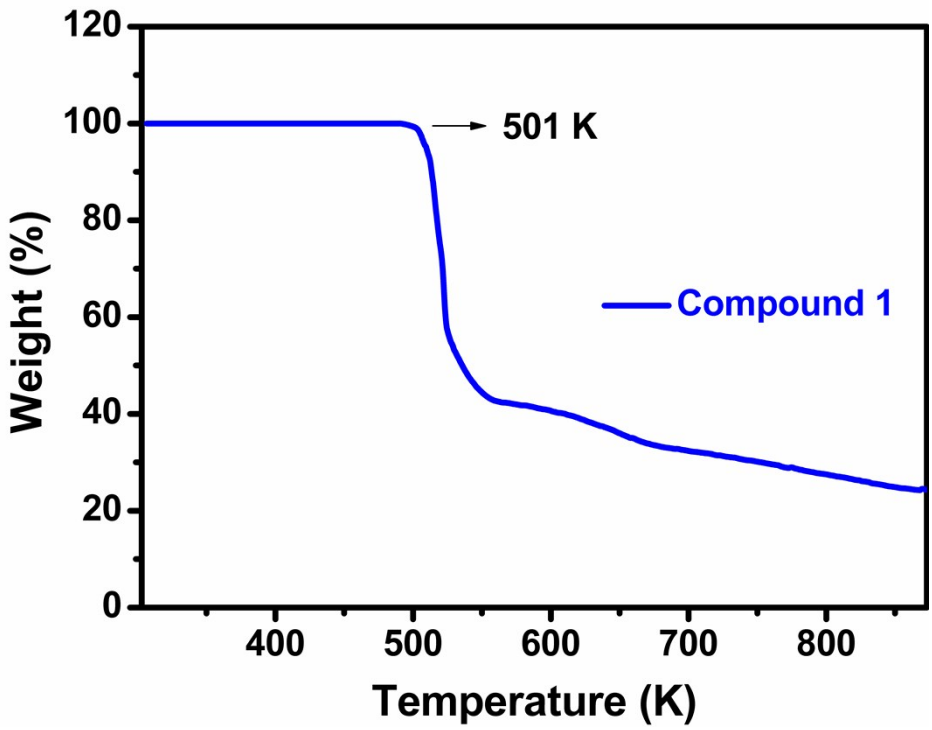

Fig. S4 TGA curve of compound **1** measured in the temperature range of 300-870 K.

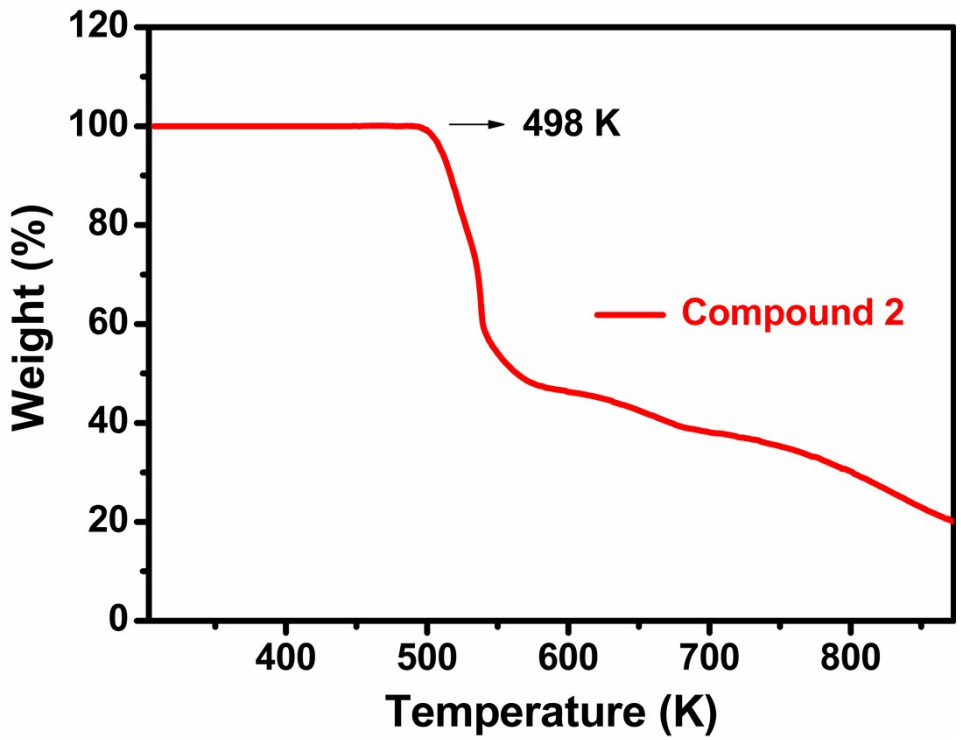

Fig. S5 TGA curve of compound **2** measured in the temperature range of 300-870 K.

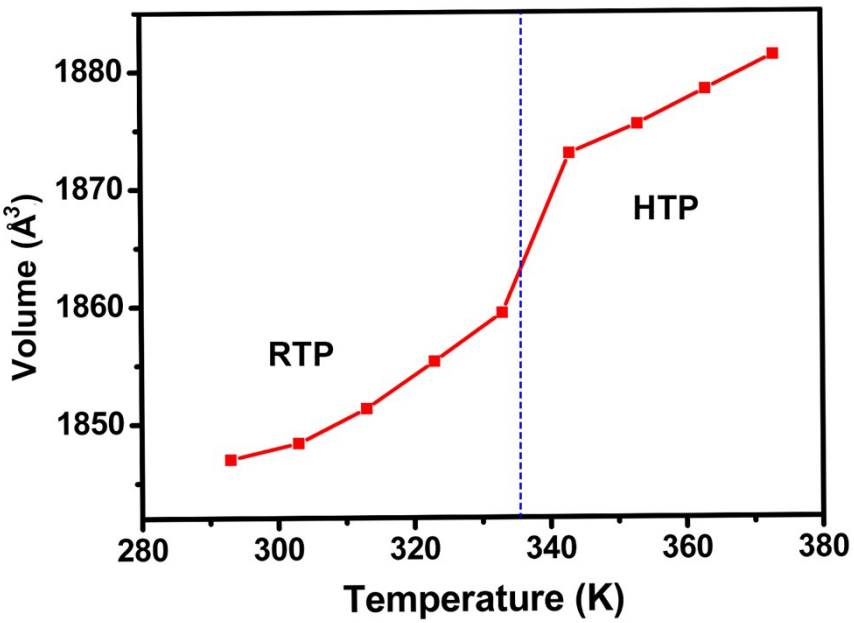

Fig. S6 The volume of compound **1** as a function of temperature.

Table S1 Selected bond lengths [Å] and angles [°] for compound **1** at 293 K

293 K	Cl(5)-C(4)	1.755(7)	Cl(6)-C(8)	1.752(7)
	Cu(1)-Cl(2)	2.236(2)	Cu(1)-Cl(3)	2.2534(19)
	Cu(1)-Cl(1)	2.248(2)	Cu(1)-Cl(4)	2.259(2)
	N(2)-C(8)-Cl(6)	112.7(5)	N(1)-C(4)-Cl(5)	112.5(4)
	Cl(2)-Cu(1)-Cl(1)	135.25(9)	Cl(2)-Cu(1)-Cl(3)	98.84(7)
	Cl(1)-Cu(1)-Cl(3)	99.82(7)	Cl(2)-Cu(1)-Cl(4)	98.56(8)
	Cl(1)-Cu(1)-Cl(4)	98.36(9)	Cl(3)-Cu(1)-Cl(4)	132.06(8)

Table S2 Selected bond lengths [Å] and angles [°] for compound **2** at 293 K

293K	C(1)-Cl(4)	1.763(2)	Cl(1)-Cu(1)	2.3299(9)
	Cl(3)-Cu(1)	2.2542(9)	Cl(1)-Cu(1)#1	2.3358(8)
	Cl(2)-Cu(1)#2	2.2860(9)	Cl(2)-Cu(1)	2.6897(11)
	Cu(1)-Cl(2)#2	2.2860(9)	Cu(1)-Cl(1)#1	2.3358(8)
	N(1)-C(1)-Cl(4)	112.38(14)		
	Cu(1)#2-Cl(2)-Cu(1)	95.82(3)	Cu(1)-Cl(1)-Cu(1)#1	96.09(3)
	Cl(3)-Cu(1)-Cl(1)	91.44(4)	Cl(3)-Cu(1)-Cl(2)#2	92.71(4)
	Cl(3)-Cu(1)-Cl(1)#1	146.27(3)	Cl(2)#2-Cu(1)-Cl(1)	175.28(2)
	Cl(1)-Cu(1)-Cl(1)#1	83.91(3)	Cl(2)#2-Cu(1)-Cl(1)#1	93.85(3)
	Cl(2)#2-Cu(1)-Cl(2)	84.18(3)	Cl(3)-Cu(1)-Cl(2)	108.72(4)
	Cl(1)#1-Cu(1)-Cl(2)	104.84(4)	Cl(1)-Cu(1)-Cl(2)	92.36(3)

Symmetry codes: #1 -x+1, -y, -z+1; #2 -x+2, -y, -z+1.

Table S3 Selected bond lengths [Å] and angles [°] for compound **2** at 343 K

343K	C(1)-Cl(4)	1.758(3)	Cu(1)-Cl(2)#1	2.2875(9)
	Cu(1)-Cl(3)	2.2607(10)	Cu(1)-Cl(1)#2	2.3452(10)
	Cu(1)-Cl(1)	2.3354(10)	Cu(1)-Cl(2)	2.7037(11)
	Cl(1)-Cu(1)#2	2.3452(10)	Cl(2)-Cu(1)#1	2.2875(9)
	N(1)-C(1)-Cl(4)	112.7(2)		
	Cl(3)-Cu(1)-Cl(2) #1	92.95(4)	Cl(3)-Cu(1)-Cl(1)	91.40(4)
	Cl(2)#1-Cu(1)-Cl(1)	175.06(4)	Cl(3)-Cu(1)-Cl(1)#2	145.96(4)
	Cl(2)#1-Cu(1)-Cl(1)#2	93.79(4)	Cl(1)-Cu(1)-Cl(1)#2	83.88(4)
	Cl(3)-Cu(1)-Cl(2)	109.01(4)	Cl(2)#1-Cu(1)-Cl(2)	83.98(3)
	Cl(1)-Cu(1)-Cl(2)	92.40(3)	Cl(1)#2-Cu(1)-Cl(2)	104.87(4)
	Cu(1)-Cl(1)-Cu(1)#2	96.12(4)	Cu(1)#1-Cl(2)-Cu(1)	96.02(3)

Symmetry codes: #1 -x, -y+1, -z+1; #2 -x+1, -y+1, -z+1.