Supporting Information

Reversible Phase Transition Driven by Order-Disorder of Metal-halide Moieties in $[(C_6H_{14})\ NH_2]_2{\bullet}CuBr_4$

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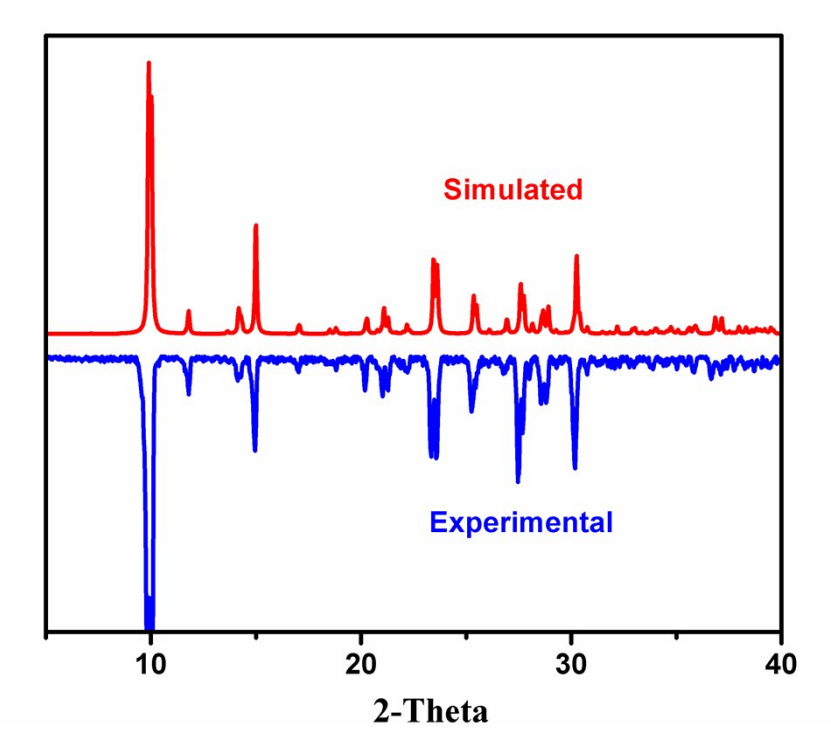

Figure S1. P-XRD pattern of compound **1**

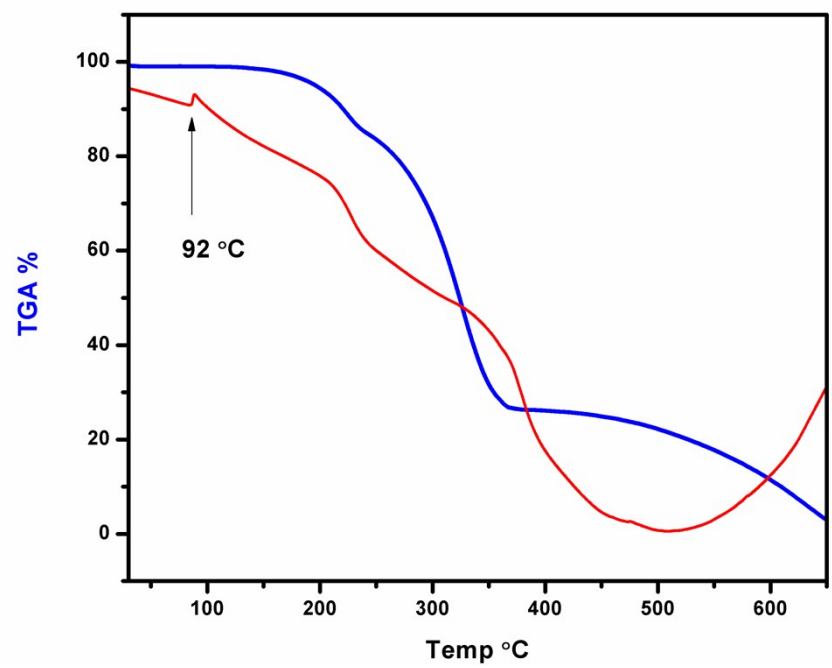

Figure S2. TG-DTA curves of compound **1**

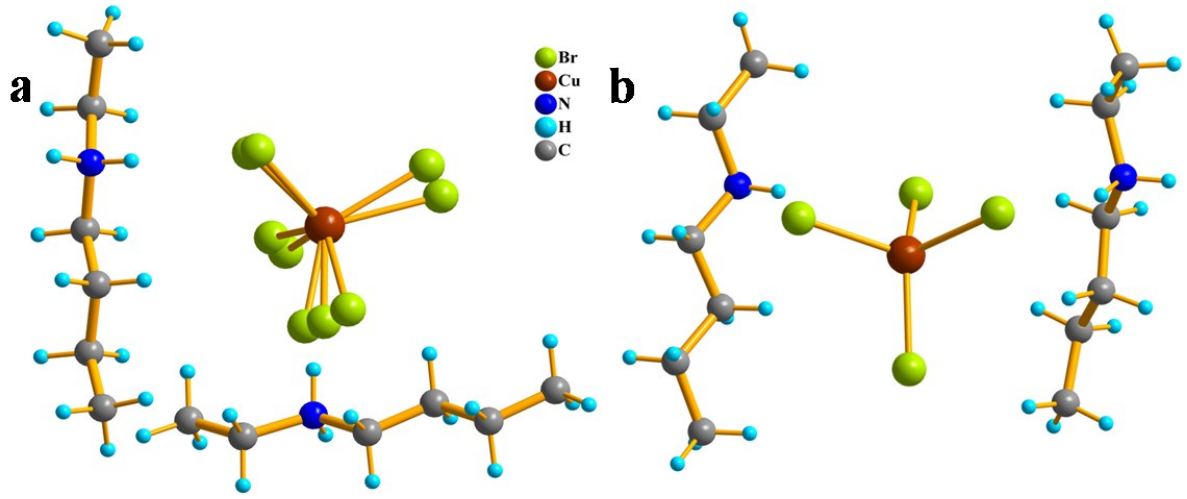

Figure S3. Asymmetric unit of **1** at HTP (a) and at LTP (b).

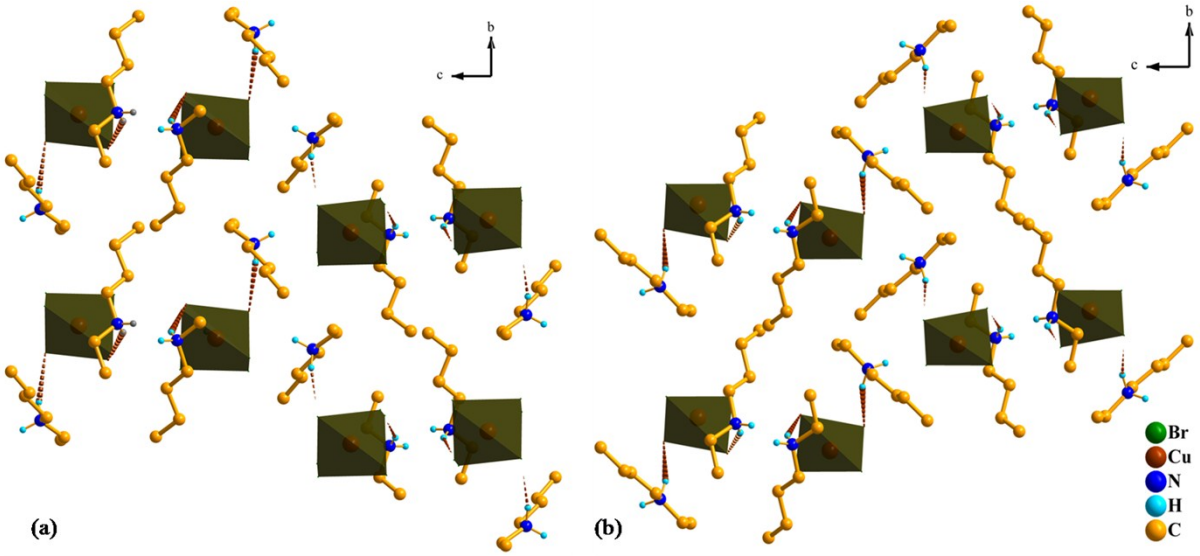

Figure S4. The packing diagram of **1** at HTP (a) and LTP (b).

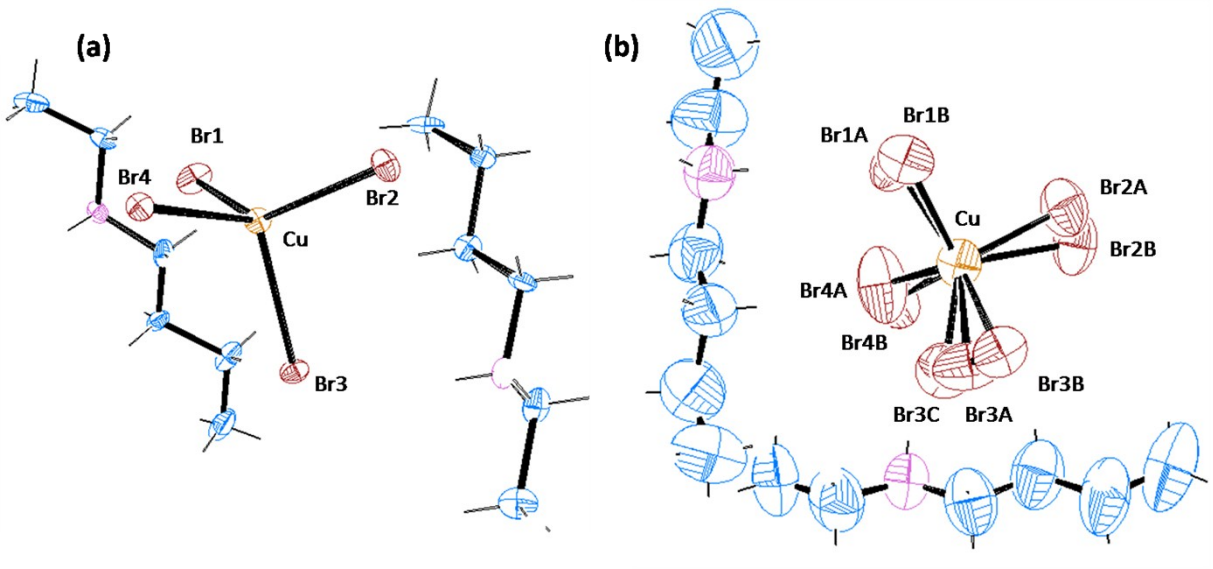

Figure S5. Thermal ellipsoidal view of **1** at (a) 120 K and (b) at 240 K after splitting of bromine atom.

Table S1. Crystal Data and structure refinement details of **1** at 120 and 240 K.

Sum formula	$C_{12}H_{32}N_2CuBr_4$	$C_{12}H_{32}N_2CuBr_4$
Formula weight	587.55	587.55
Temperature (K)	120	240
Crystal system	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
a/Å	9.4138	9.4357
b/Å	9.4206	9.5934
c/Å	23.8513	24.6862
α/deg	90	90
β/deg	90	90
γ/deg	90	90
Volume (Å^3)	2115.22	2234.61
Z	4	4
D_{calcd}, g cm^{-1}	1.845	1.745
F(000)	1148	1148
Completeness (%)	99.6	99.8
Goodness-of-fit on F^2	1.038	1.056
R_1 (on F_o^2, $I>2\sigma(I)$)	0.034	0.034
wR_2 (on F_o^2, $I>2\sigma(I)$)	0.081	0.081

$\alpha R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma(|F_o|^2 - |F_c|^2) / \Sigma|F_o|^2]^{1/2}$