Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Importing spontaneous polarization into a Heisenberg ferromagnet for a potential single-phase multiferroic

Bo Huang,[a] Bao-Ying Wang,[a] Zi-Yi Du,[b] Wei Xue,[a] Wei-Jian Xu,[a] Yu-Jun Su,[a] Wei-Xiong Zhang,*[,a] Ming-Hua Zeng,[c] and Xiao-Ming Chen[a]

[a.] MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry & Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, China. E-mail: zhangwx6@mail.sysu.edu.cn

[b.] College of Chemistry and Chemical Engineering, Gannan Normal University, Ganzhou 341000, China

[c.] School of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, Guilin 541004, China.

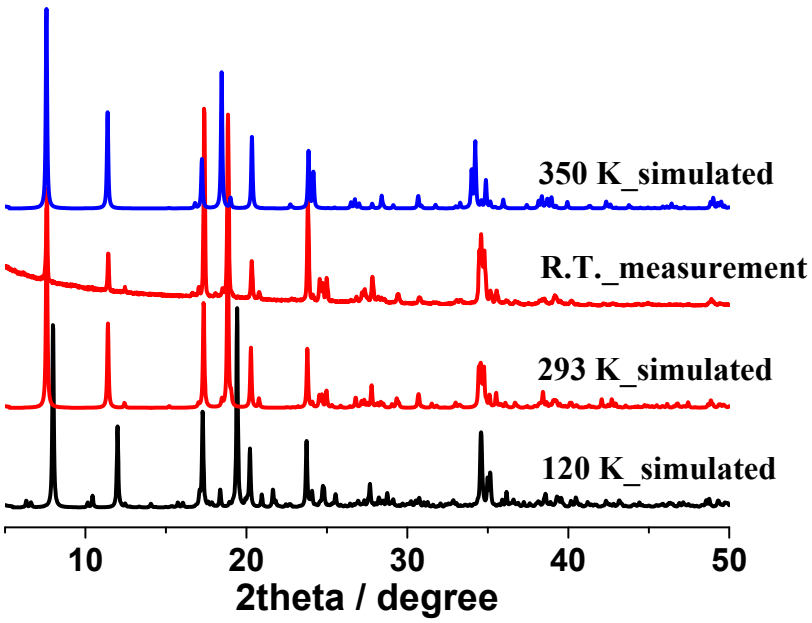

Fig. S1 The experimental powder XRD pattern at room temperature compared to the simulated one at 120 K, 293 K and 350 K.

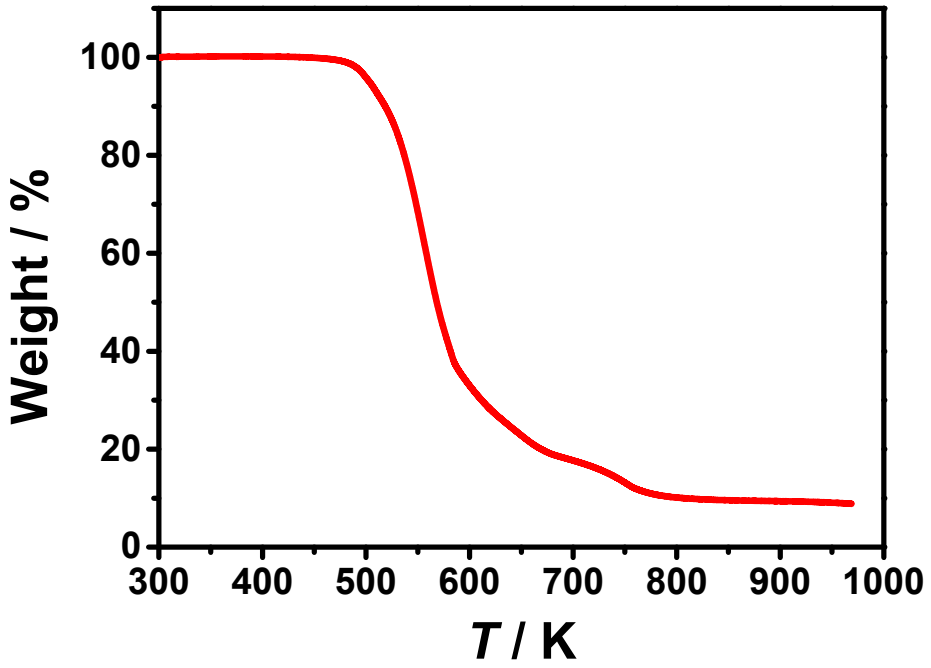

Fig. S2 Thermogravimetric analysis curve at a rate of 5 K/min under N_2 atmosphere.

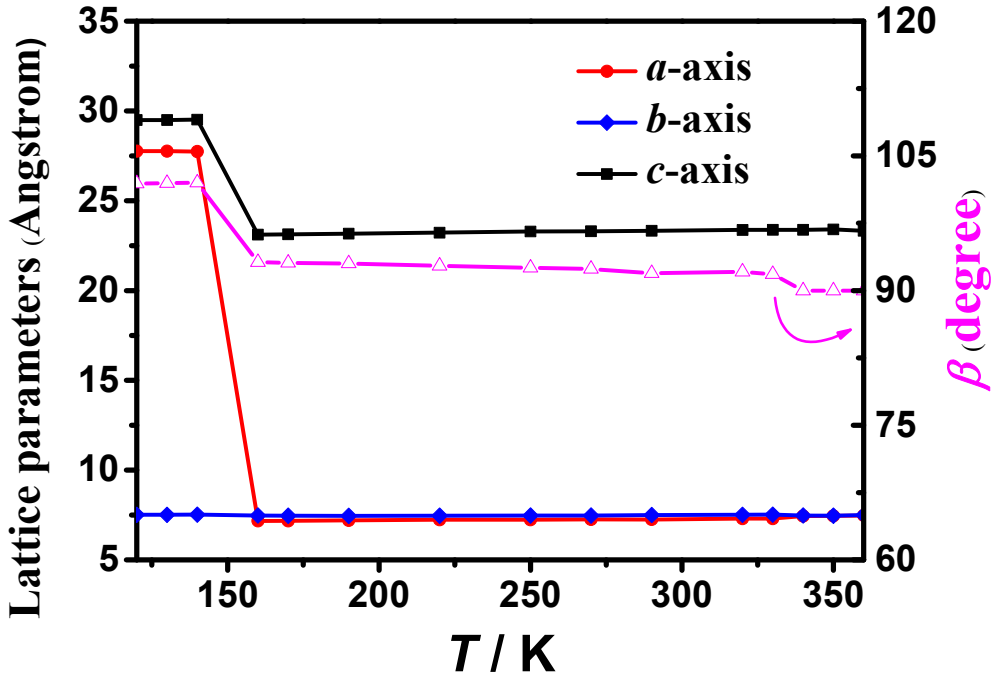

Fig. S3 *In situ* variable-temperature measurements for the cell parameters.

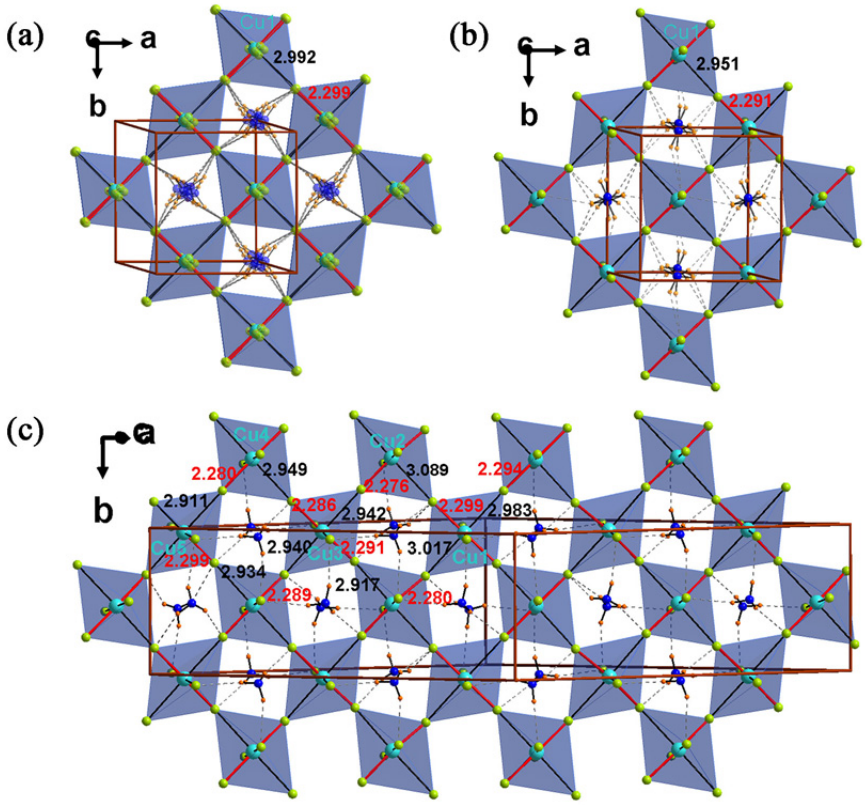

Fig. S4 Layers of corner-sharing Jahn-Teller distorted $CuC1_6$ octahedra at 350 K (a), 293 K (b), and 120 K (c). Cu, Cl, N, and H atoms are shaded in aqua, lime, blue and gold, respectively. Hydrogen bonds are represented by dashed lines. The length of the long (black)/short bonds (red) of the $CuCl_6$ octahedron is 2.992/2.299 Å at 350 K, 2.951/2.291 Å at 293 K, and 2.911–3.089/2.276–2.299 Å at 120 K, respectively.

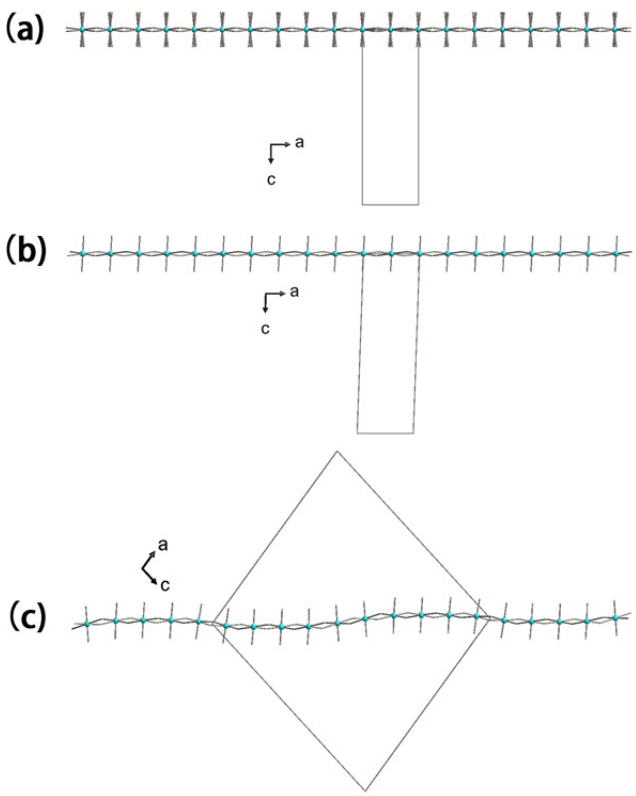

Fig. S5 The inorganic layer of **1** at 350 K (a), 293 K (b) and 120 K (c).

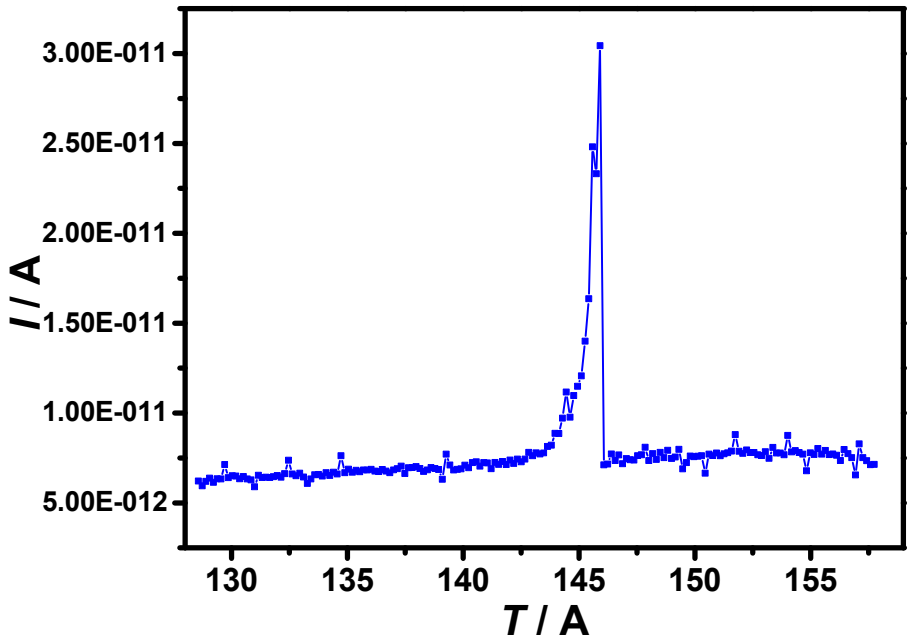

Fig. S6 The pyroelectric current in the vicinity of the ferroelectric phase transition.

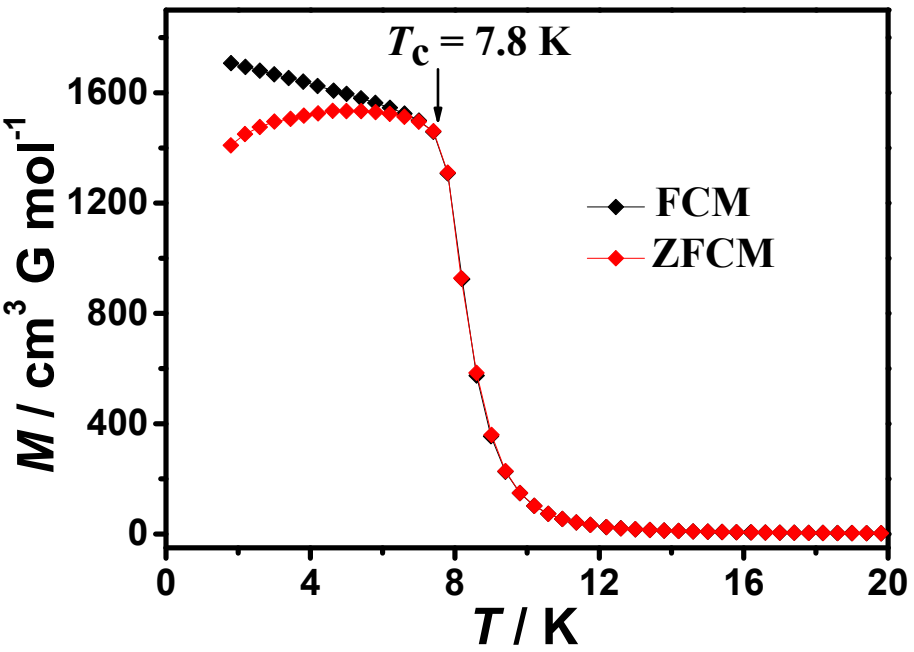

Fig. S7 Zero-field-cooled magnetization and field-cooled magnetization of **1**.