Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Molecular Ferroelectric Pyridin-2-ylmethanaminium Perchlorate with Phase Transition Induced by Disorder of Perchlorate

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Table S1. Crystal data and geometry details of compound **1.**

	The LTP	The HTP
Chemical formula	$C_6 H_{10} Cl_2 N_2 O_8$	$C_6 H_{10}Cl_2 N_2O_8$
Mr	309.06	309.06
Space group	P 2_1	P $2_1/c$
Temperature (K)	173K	293K
a (Å)	11.7656(10)	11.868(7)
b (Å)	15.0880(1)	15.208(9)
c (Å)	13.1523(10)	13.240(8)
β	91.7930(5)	92.470(9)
Volume (Å3)	2333.7(3)	2387(2)
Z	8	8
R, wR2, S	0.1085, 0.3512, 1.173	0.0856, 0.2727, 0.890
Bond length (Å)	LTP	HTP
C1-C2	1.327(15)	1.351(7)
C2-C3	1.411(18)	1.365(9)
C3-C4	1.360(16)	1.374(7)
C4-C5	1.394(15)	1.378(6)
C1-N1	1.380(13)	1.352(6)
C5-N1	1.329(12)	1.321(5)
C5-C6	1.501(14)	1.506(5)
C6-N2	1.475(13)	1.496(5)
C7-C8	1.426(15)	1.329(8)
C8-C9	1.293(17)	1.341(8)
C9-C10	1.452(16)	1.491(9)
C10-C11	1.373(16)	1.353(7)
C7-N3	1.321(13)	1.332(7)
C11-N3	1.312(15)	1.333(6)
C11-C12	1.508(15)	1.504(6)
C12-N4	1.539(12)	1.497(5)
Bond angle(º)	LTP	HTP

C1-C2-C3	118.4(5)	118.2(4)
C2-C3-C4	120.7(6)	120.0(4)
C3-C4-C5	119.1(6)	120.6(4)
C4-C5-N1	118.0(5)	117.6(4)
N1-C1-C2	119.9(6)	120.8(4)
C1-N1-C5	122.9(5)	122.7(4)
C4-C5-C6	119.8(5)	124.0(3)
N1-C5-C6	121.8(5)	118.3(3)
C5-C6-N2	109.5(5)	110.2(3)
C7-C8-C9	119.4(5)	122.6(4)
C8-C9-C10	122.4(6)	118.0(4)
C9-C10-C11	117.1(6)	116.4(4)
C10-C11-N3	115.9(6)	119.5(4)
N3-C7-C8	114.4(6)	118.2(4)
C7-N3-C11	130.0(6)	124.9(4)
C10-C11-C12	125.7(6)	123.7(4)
N3-C11-C12	118.3(5)	116.8(3)
C11-C12-N4	108.3(5)	111.1(3)

Table S2. The frequency-dependent Curie constants of Curie-Weiss law of the heating process.

Frequency	C_{para}(K)	C_{ferro}(K)
500Hz	68	250
1 kHz	76	256
5kHz	120	345
10kHz	118	263
100kHz	150	416
1 MHz	263	526

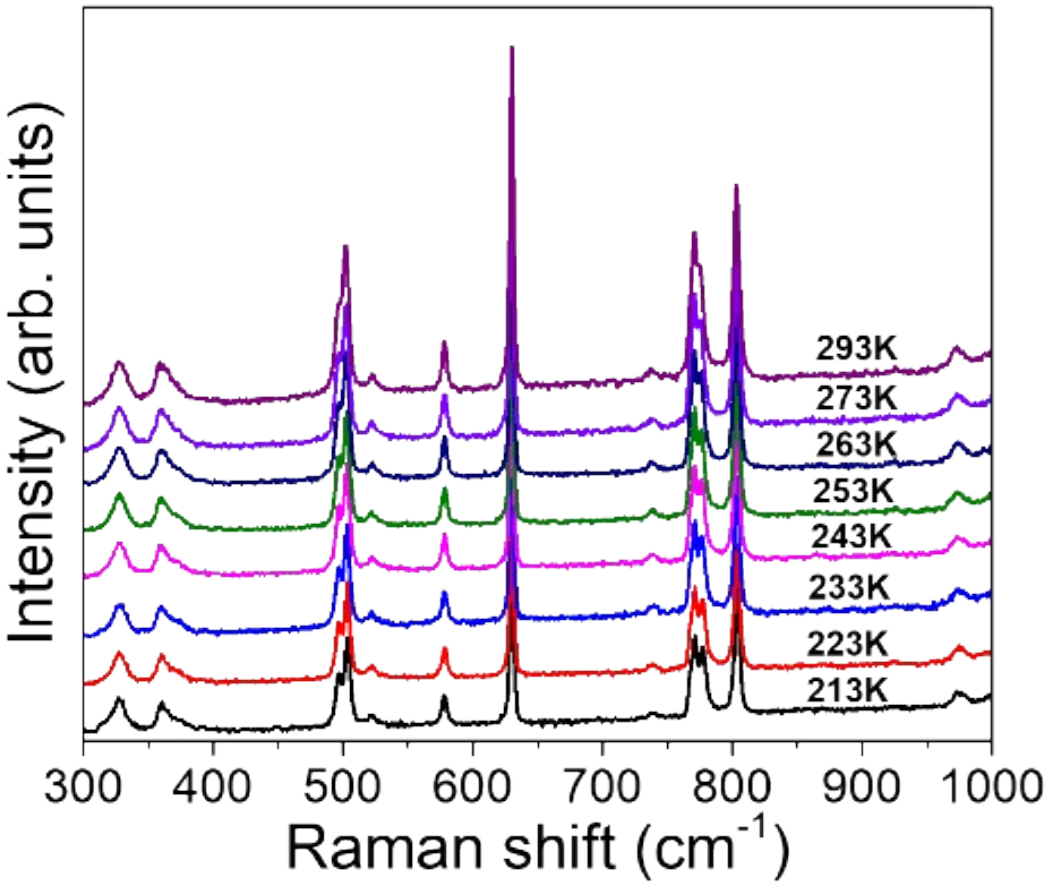

Figure S1. Raman spectra of compound 1 within the selected wavenumber range at different temperatures.

In order to understand the phase transition mechanism, the temperature evolution of Raman spectra has been conducted cooling down from room temperature to 213 K. Figure S1 presents the Raman spectra in the frequents range of 300–1000 cm^{-1} in cooling process.

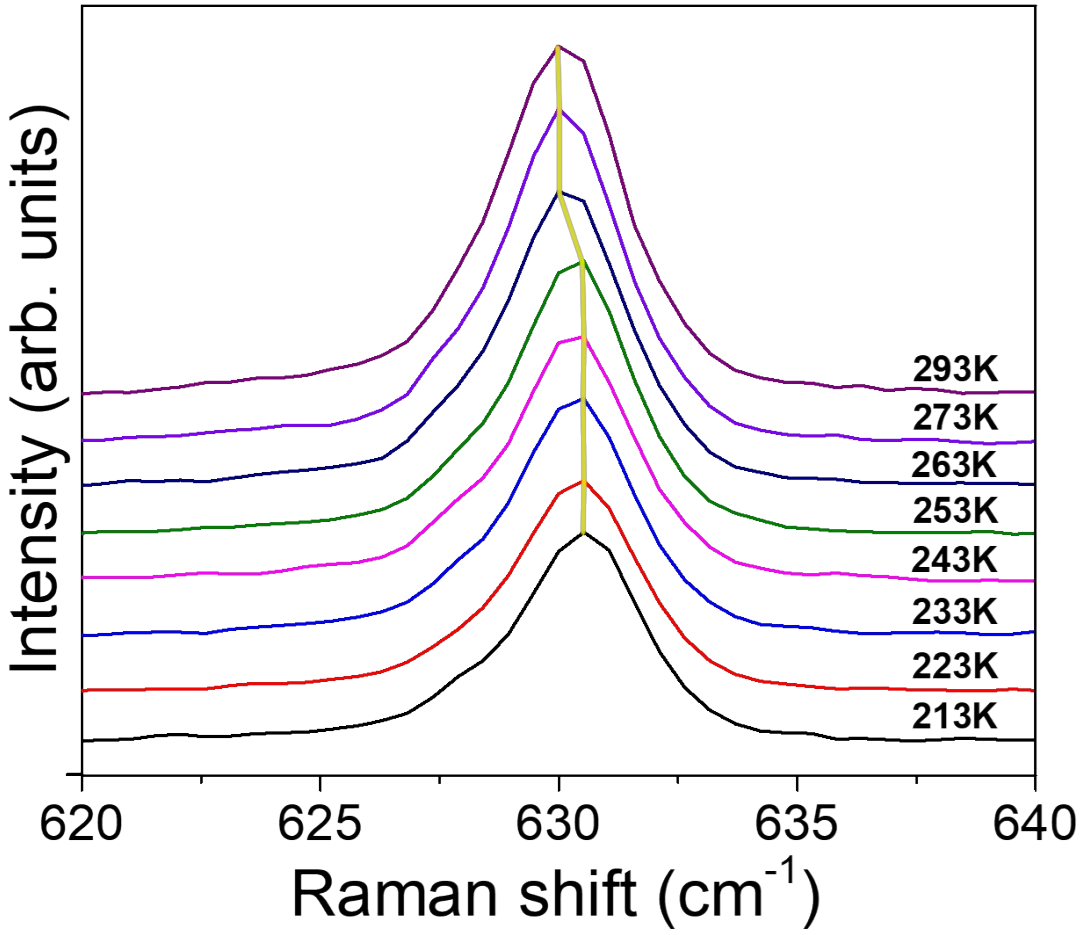

Figure S2. Raman peak position shifts at 628 cm^{-1} at different temperatures.

Since the vibration at 628 cm^{-1} comes from the inplane deformation of the perchlorate anion. By variable temperature Raman peak position shifts before and after the phase transition at 628 cm^{-1}, it can also be seen that the change of Raman peak position shifts before and after the phase transition. In other words, the disorder of perchloric acid changes before and after the phase transition.