Supporting Information

Ferroelastic Phase Transition and Dielectric Anomalies in 2, 4, 6-Trimethylanilinium Perchlorate

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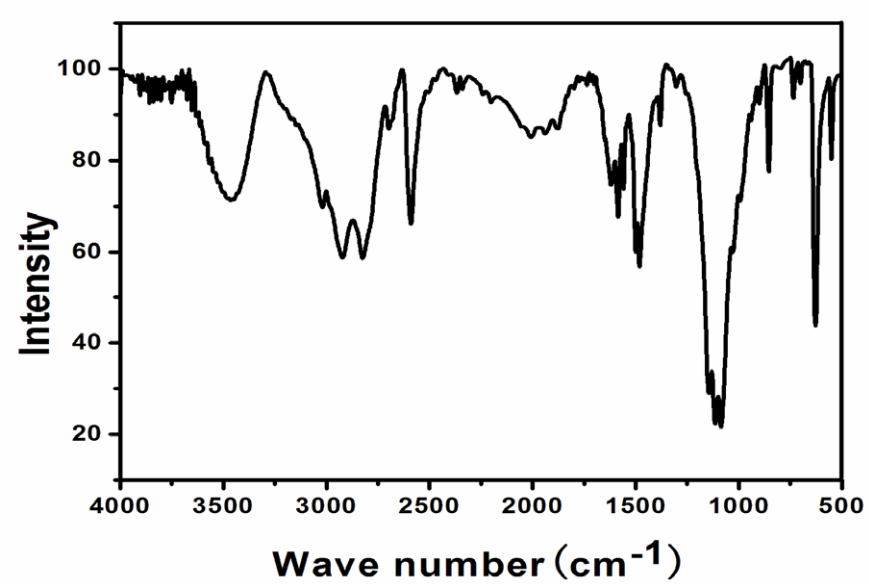

Figure 1S. IR of compound **1**

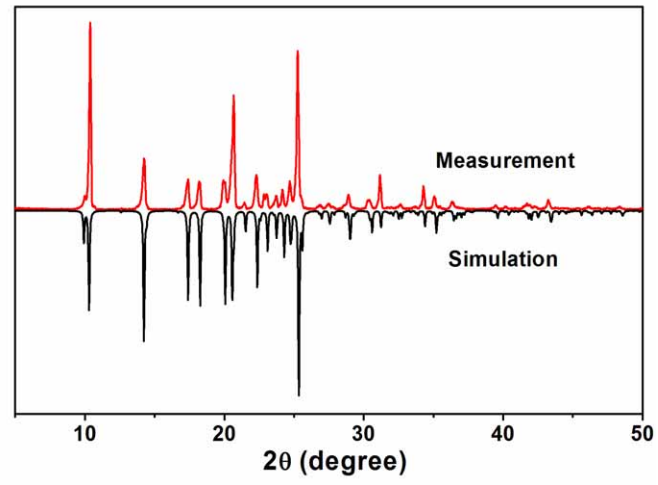

Figure 2S. X-ray powder diffraction (XRPD) of compound **1**.

Table 1s. Crystal data of compound **1**.

Empirical formula	$C_9H_{14}NClO_4$	$C_9H_{11}NClO_4$
Formula weight	235.66	232.64
T/ ^{O}C	25(2)	110(2)
Crystal system	triclinic	monoclinic
space group	*P*-1	$P2_1/m$
a / Å	7.1581(14)	8.9084(18)
b / Å	8.5937(17)	7.2253(18)
c / Å	9.0642(18)	9.172(3)
V / Å^3	546.90(19)	587.6(3)
α / º	88.74(3)	90
β / º	79.19(3)	95.55(3)
γ / º	87.02(3)	90
Z	2	2
D_{cal} / (Mg/m^3)	1.431	1.315
μ / mm^{-1}	0.344	0.319
Reflections collected	5745	5664
Reflections unique	2506	1444
Data / restraints / parameters	2506 / 7 / 140	1444 / 0 / 91
Goodness-of-fit on F^2	1.076	1.394
Largest diff. peak and hole / e·Å^{-3}	0.850 and -1.036	0.556 and -0.457
R indices [*I*>2sigma(*I*)]	R_1 = 0.0790	R_1 = 0.1120
	wR_2 = 0.2001	wR_2 = 0.3461
R indices (all data)	R_1 = 0.0979	R_1 = 0.1487
	wR_2 = 0.2151	wR_2 = 0.3862

Table 2s. Hydrogen-bond geometry(Å, °) in compound **1**

25 ^{O}C	D–H	H···A	D···A	D–H···A
N1-H1A···O1^{i}	0.8900	2.2000	2.976(5)	144.900
N1-H1C···O3^{ii}	0.8900	2.1600	2.969(5)	150.500
N1-H1B···O2	0.8900	2.1500	2.974(5)	154.400
C9-H9B···Cg	0.9600	2.9946	3.7635	138.03
110 ^{O}C				
N1-H1A···O2^{iii}	0.7000	2.4400	3.046(12)	145.700
N1-H1B···O1^{iv}	0.9500	2.3200	2.990(12)	126.700
N1-H1C···O1^{v}	0.9500	2.3200	2.990(12)	126.700

Symmetry codes: (i) 1-x, 1-y, -z; (ii) 1+x, y, z; (iii) 1-x, 0.5-y, 1-z; (iv) x, y, z+1; (v) x, 0.5-y, 1+z

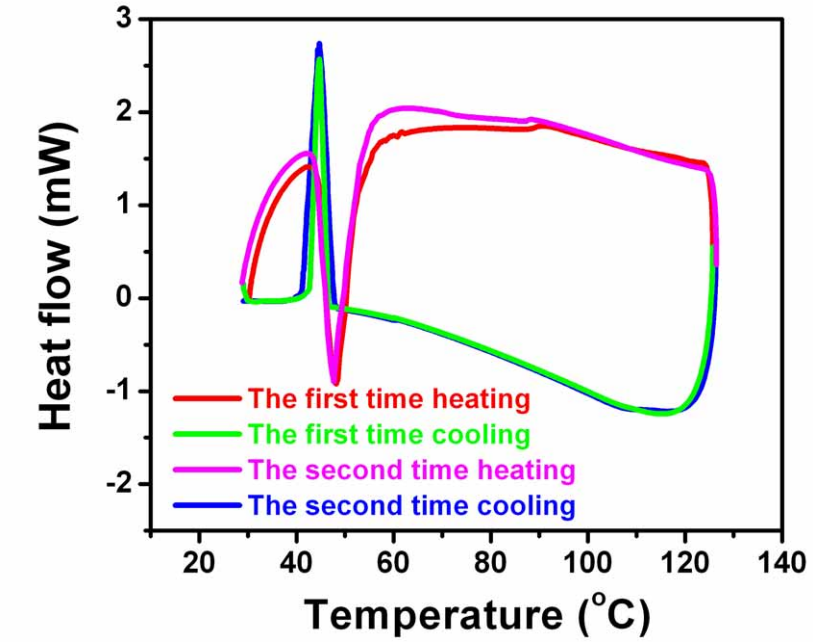

Figure S3 DSC diagram of compound **1** running two cycles.