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Supporting Information

High-temperature molecular ferroelastic phase transition and switchable dielectric response in the trimethylbromomethylammonium salt $[C_4H_{11}NBr]$ $[PF_6]$

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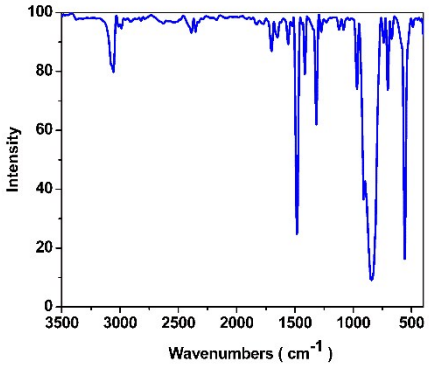

Figure S1. Infrared (IR) spectra of solid **1** in KBr pellet recorded on a Shimadzu model IR-60 spectrometer at room temperature.

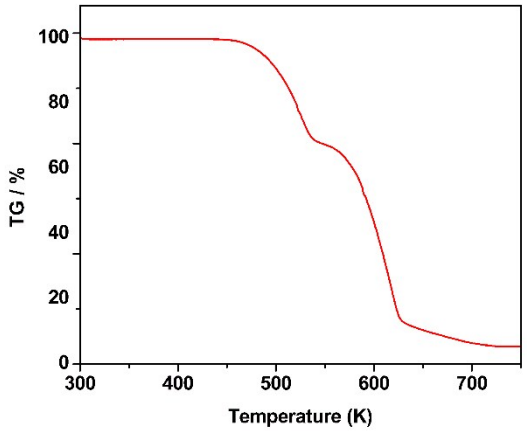

Figure S2. Thermal analysis for **1**, revealing the good thermal stability up to 450 K.

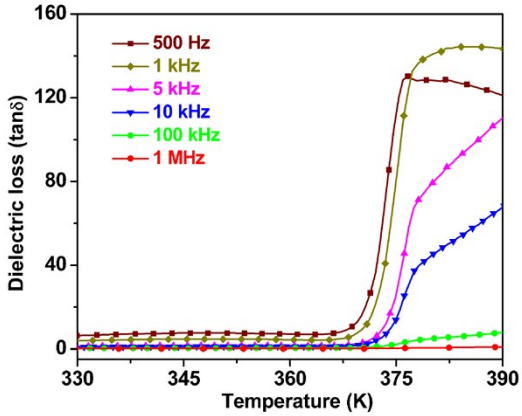

Figure S3. The temperature-dependence of dielectric loss (tanδ) of **1** measured at selected frequencies (500 Hz-1 MHz).

Table S1 Selected geometric parameters (Å, °)

Br1—C1	1.927 (8)	F2—P1	1.564 (6)
C1—N1	1.463 (9)	F3—P1	1.568 (6)
C2—N1	1.486 (10)	F4—P1	1.572 (5)
C3—N1	1.502 (9)	F5—P1	1.566 (6)
C4—N1	1.504 (9)	F6—P1	1.564 (6)
F1—P1	1.551 (6)		
N1—C1—Br1	112.8 (5)	F2—P1—F5	178.5 (4)
C1—N1—C2	106.7 (6)	F6—P1—F5	92.7 (4)
C1—N1—C3	110.2 (6)	F1—P1—F3	88.9 (4)
C2—N1—C3	111.0 (6)	F2—P1—F3	91.5 (4)
C1—N1—C4	111.5 (6)	F6—P1—F3	178.1 (4)
C2—N1—C4	108.7 (7)	F5—P1—F3	87.6 (4)
C3—N1—C4	108.7 (6)	F1—P1—F4	178.6 (4)
F1—P1—F2	88.9 (4)	F2—P1—F4	90.9 (4)
F1—P1—F6	93.0 (4)	F6—P1—F4	88.4 (4)
F2—P1—F6	88.2 (4)	F5—P1—F4	88.0 (4)
F1—P1—F5	92.2 (4)	F3—P1—F4	89.7 (4)

Table S2 Summary of the analysis of the phase transition on TMHMA-based compounds

Compound	T_c/K	ordered-disordered part for phase transition
[TMCM-$MnCl_3$]	406	[TMCM] cations
[TMCM-$CdCl_3$]	400	[TMCM] cations
[TMBM-$MnBr_3$]	415	[TMBM] cations
[TMBMA][PF_6]	**380**	