Electronic Supplementary Materials (ESI)

Dielectric Switch of High Temperature Plastic Phase Transition in Two Organic Salts with Chiral Feature

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1. Synthetic scheme of precursor, compound 1 and compound 2

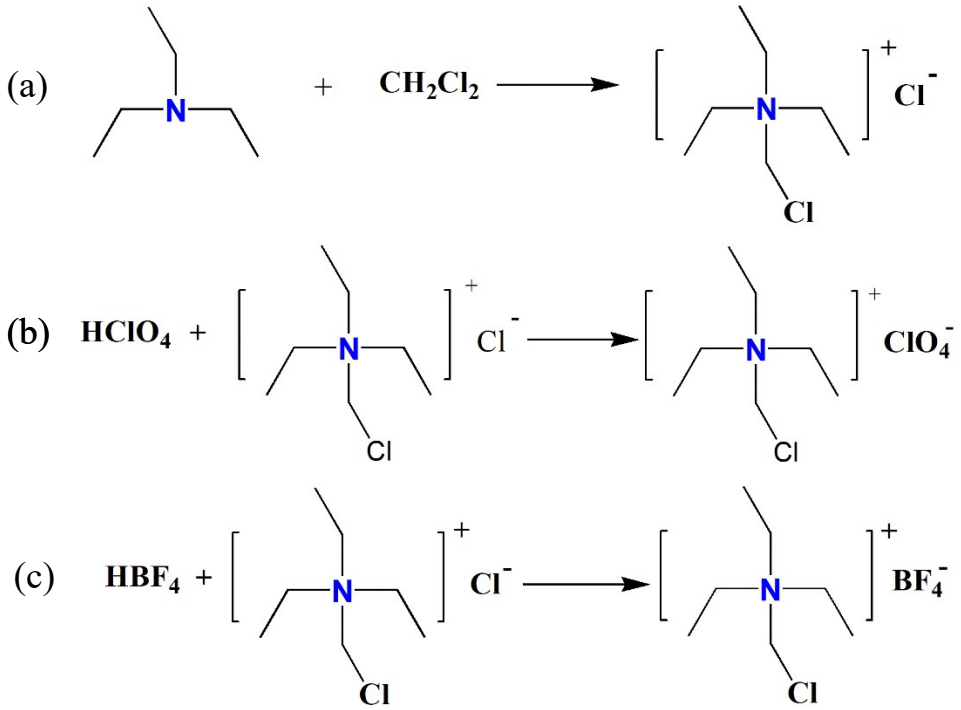


Figure S1. Schematic diagrams of synthesis of precursor(a), compounds **1**(b) and **2**(c).

2. Infrared spectra of compounds 1 and 2

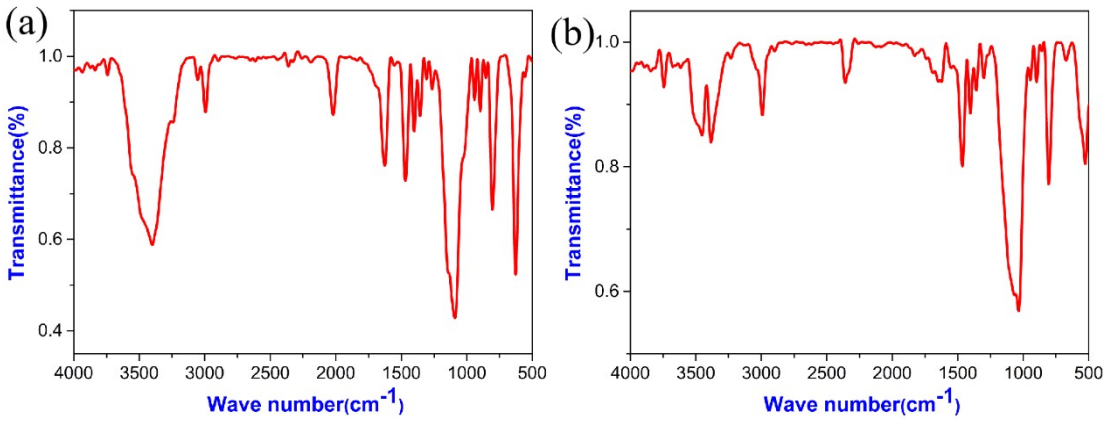


Figure S2. Infrared spectra of compounds **1**(a) and **2**(b)

3. Thermogravimetric analysis (TGA) of compounds 1 and 2

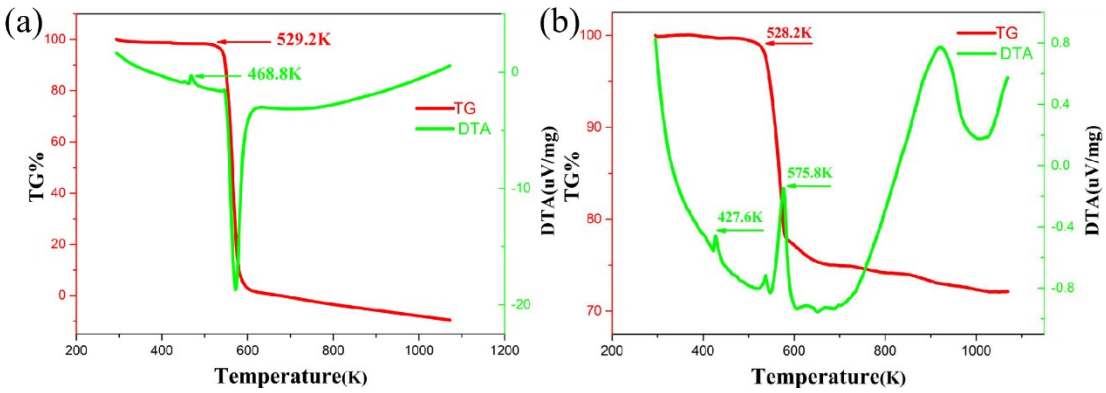
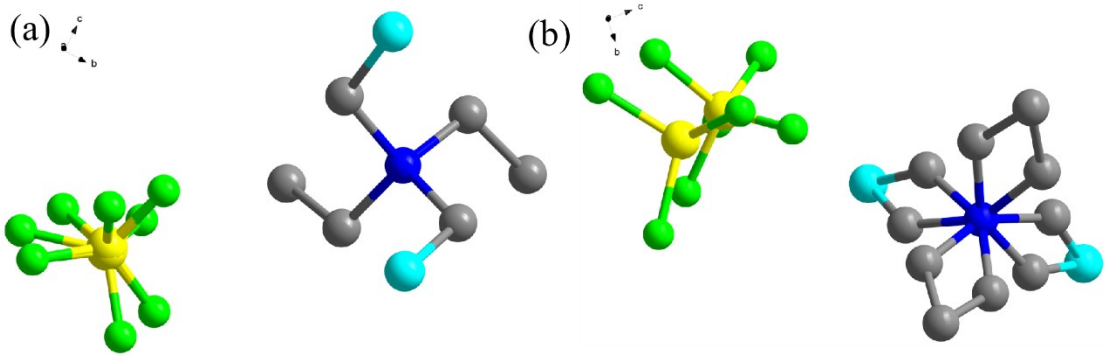


Figure S3. TGA diagram for compounds **1**(a) and **2**(b)

4. I-Phase(a) and II-Phase(b) and III-Phase(c) of compound 2 coordination environment map; II-Phase(d) of compound 2 stacked graph along the C axis.



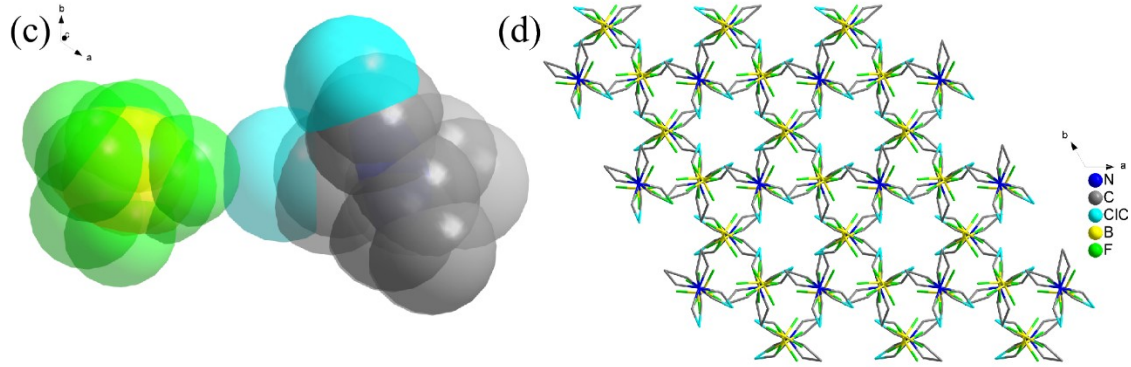


Figure S4. I-Phase(a) and II-Phase(b) and III-Phase(c) of compound **2** coordination environment map; II-Phase(d) of compound **1** stacked graph along the C axis.

5. Summary of the crystallographic data for crystal of 1 and 2

Table S1. Summary of the crystallographic data for crystal of **1** and **2**

compound	**1-I**	**1-II**	**2-I**	**2-II**
Empirical formula	$C_7Cl_2NO_4$	$C_7Cl_2NO_4$	$BClC_7F_4N$	$BClC_7F_4N$
Formula weight	232.98	232.98	220.34	220.32
Temperature	293 K	430 K	293 K	420 K
Crystal system	Trigonal	Trigonal	Trigonal	Trigonal
Space group	$P3_221$	$P3_121$	$P3_221$	$P3_221$
a (Å)	7.3426(3)	7.4295(4)	7.2791(3)	7.3906(6)
b (Å)	7.3426(3)	7.4295(4)	7.2791(3)	7.3906(6)
c (Å)	19.3196(10)	19.6225(13)	19.0645(11)	19.390(2)
V (Å^3)	902.05(9)	940.53(12)	874.80(9)	917.2(18)
D_{calca}/Mg·m^{-3}	1.287	1.234	1.255	1.197
Z	3	3	3	3
μ (mm^{-1})	0.528	0.506	0.340	0.324
GOF	1.731	1.514	1.469	3.047
$R1[I > 2\sigma(I)]$	R_1= 0.1301, wR_2 =0.4029	R_1 = 0.1548, wR_2 =0.3959	R_1=0.1222, wR_2=0.3613	R_1 = 0.3927, wR_2 = 0.7417
$wR2$ (all data)	R_1 = 0.1474, wR_2 =0.4134	R_1 = 0.1947, wR_2= 0.4295	R_1=0.1455, wR_2=0.3828	R_1 = 0.4516, wR_2= 0.7710
$\Delta\rho$max/$\Delta\rho$min(e Å^{-3})	0.65 /-1.01	0.65 /-0.75	0.64 /-0.37	1.76/-0.97

6. Calculation of ΔS and N for compounds 1 and 2

(1) Compound 1:

In the I/II phase cooling cycle mode：

$$\Delta S_1 = R\ln N_1 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{3.371 J.g^{-1} \cdot mol^{-1} \times 24}{397.6K} = 2.120 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_1 = exp(\frac{\Delta S_1}{R}) = exp(\frac{2.12 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}) = 1.290$$

In the I/II phase heating cycle mode：

$$\Delta S_2 = R\ln N_2 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{3.507 J.g^{-1} \cdot mol^{-1} \times 249.}{401.2K} = 2.180 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_2 = exp(\frac{\Delta S_2}{R}) = exp(\frac{2.180 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}) = 1.300$$

In the II/ III phase cooling cycle mode：

$$\Delta S_3 = R\ln N_3 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{22.83 J.g^{-1} \cdot mol^{-1} \times 249.}{417.7K} = 13.66 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_3 = exp(\frac{\Delta S_3}{R}) = exp(\frac{13.66 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}) = 5.160$$

In the II/ III phase heating cycle mode：

$$\Delta S_4 = R\ln N_4 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{21.42 J.g^{-1} \cdot mol^{-1} \times 249.}{455.2K} = 11.76 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_4 = exp(\frac{\Delta S_4}{R}) = exp(\frac{11.76J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}) = 4.110$$

(2) Compound 2:

In the I/II phase cooling cycle mode：

$$\Delta S_5 = R\ln N_5 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{3.544J.g^{-1} \cdot mol^{-1} \times 272.}{401.4K} = 2.410J \cdot mol^{-1} \cdot K^{-1}$$

$$N_5 = exp(\frac{\Delta S_5}{R}) = exp(\frac{2.410J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}) = 1.340$$

In the I/II phase heating cycle mode：

$$\Delta S_6 = R\ln N_6 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{2.997J.g^{-1} \cdot mol^{-1} \times 272.}{407.4K} = 2.010J \cdot mol^{-1} \cdot K^{-1}$$

$$N_6 = exp(\frac{\Delta S_6}{R}) = exp(\frac{2.010J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}) = 1.270$$

In the II/ III phase cooling cycle mode：

$$\Delta S_7 = R\ln N_7 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{53.79J.g^{-1} \cdot mol^{-1} \times 272.}{417.7K} = 35.13J \cdot mol^{-1} \cdot K^{-1}$$

$$N_7 = exp(\frac{\Delta S_7}{R}) = exp(\frac{35.13J \cdot mol^{-1} \cdot K^{-1}}{8.314J \cdot mol^{-1} \cdot K^{-1}}) = 68.40$$

In the II/ III phase heating cycle mode：

$$\Delta S_8$$

$$= R\ln N_8 = \int_{T_2}^{T_1} \frac{Q}{T} dT \approx \frac{\Delta H}{T_c} = \frac{55.08 J.g^{-1} \cdot mol^{-1} \times 27}{432.8 K}$$

$$= 34.71 J \cdot mol^{-1} \cdot K^{-1}$$

$$N_8 = exp(\frac{\Delta S_8}{R}) = exp(\frac{34.71 J \cdot mol^{-1} \cdot K^{-1}}{8.314 J \cdot mol^{-1} \cdot K^{-1}}) = 65.10$$