Supporting Information

$[C_7H_{14}NO][ClO_4]$: order-disorder structural change induced sudden switchable dielectric behaviour at room temperature†

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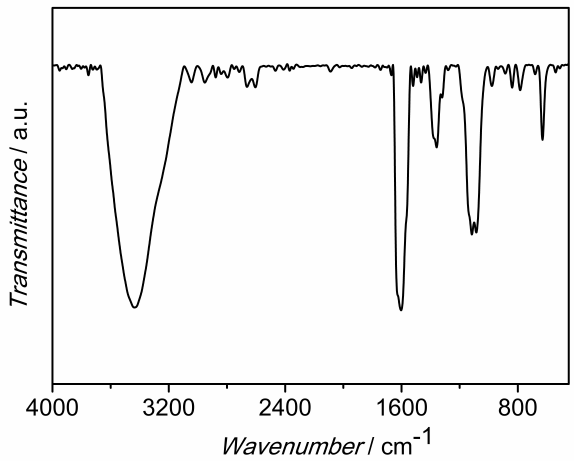

Fig. S1. IR spectra of **1** measured at room temperature.

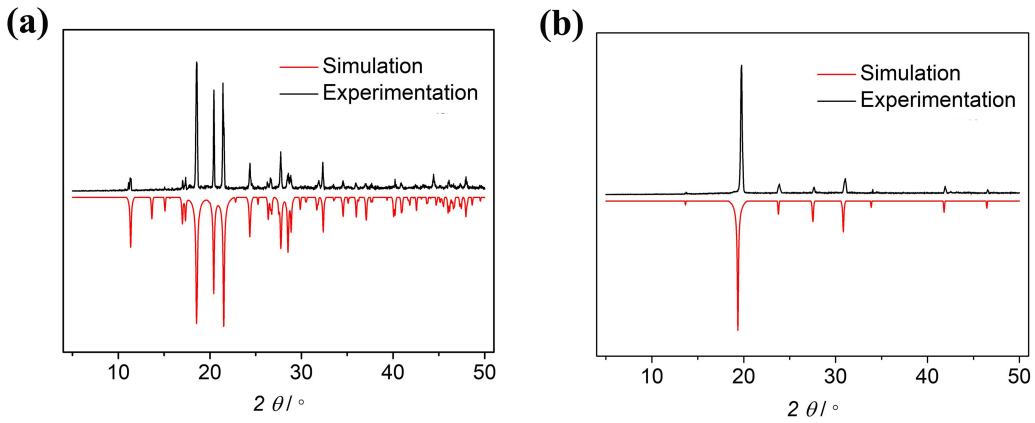

Fig. S2. PXRD patterns of **1** measured at (a) LTP and (b) HTP.

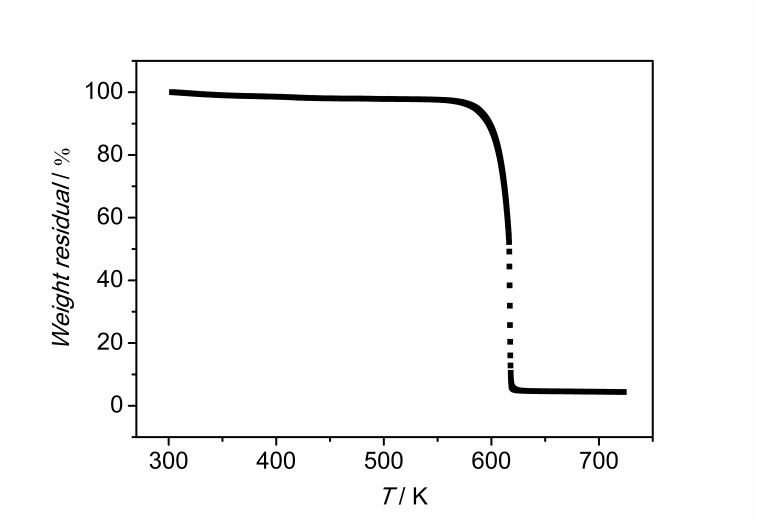

Fig. S3. TGA curve of **1**.

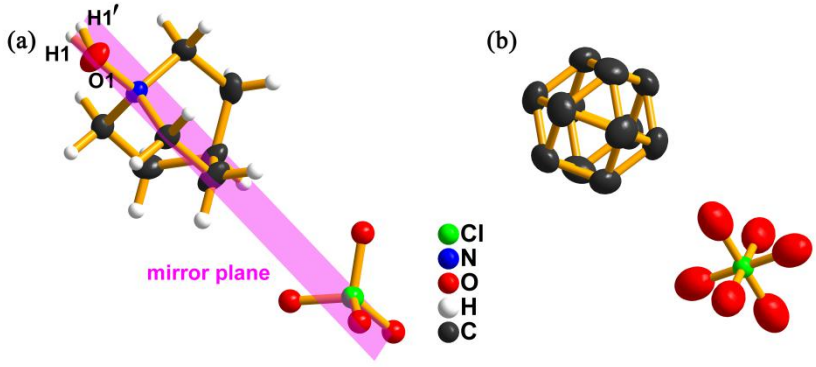

Fig. S4. The molecular structures of **1** at (a) LTP and (b) HTP.

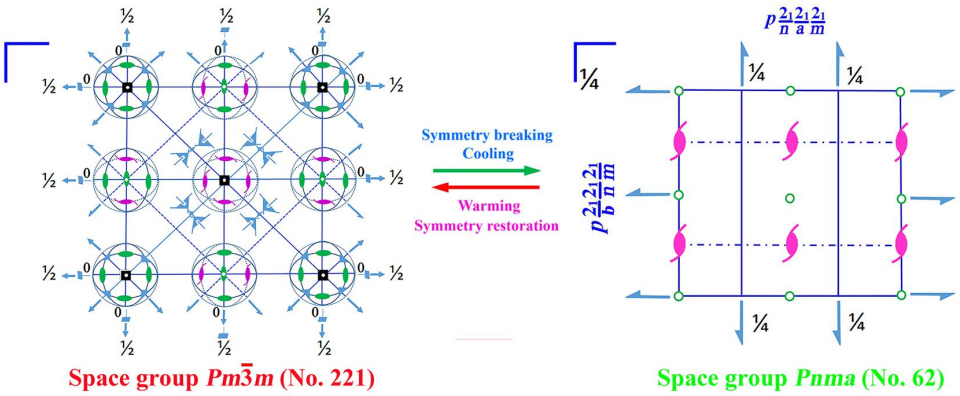

Fig. S5. Symmetry breaking in **1** from HTP ($Pm\bar{3}m$) to LTP (*Pnma*).

Table S1. Bonds lengths (Å) and angles (°) for **1**.

1 (223 K)			
Cl1−O2	1.385(7)	O2−Cl1−O3	110.4(6)
Cl1−O2#1	1.385(7)	O2−Cl1−O2#1	102.6(8)
Cl1−O3	1.419(7)	O2#1−Cl1−O3	110.4(6)
Cl1−O4	1.336(8)	O4−Cl1−O2	114.1(6)
		O4−Cl1−O2#1	114.1(6)
		O4−Cl1−O3	105.4(5)
Symmetry codes: #1 x, −y+1/2, z.			
1 (353 K)			
Cl1−O1	1.35(4)	O1−Cl1−O1#1	90.000(1)
Cl1−O1#1	1.35(4)	O1−Cl1−O1#2	90.000(1)
Cl1−O1#2	1.35(4)	O1−Cl1−O1#3	180.0
Cl1−O1#3	1.35(4)	O1−Cl1−O1#4	90.0
Cl1−O1#4	1.35(4)	O1−Cl1−O1#5	90.0
Cl1−O1#5	1.35(4)	O1#1−Cl1−O1#2	180.0
		O1#1−Cl1−O1#3	90.000(1)
		O1#1−Cl1−O1#4	90.000(1)
		O1#1−Cl1−O1#5	90.000(1)
		O1#2−Cl1−O1#3	90.000(1)
		O1#2−Cl1−O1#4	90.000(1)
		O1#2−Cl1−O1#5	90.000(1)
		O1#3−Cl1−O1#4	90.000(1)
		O1#3−Cl1−O1#5	90.000(1)
		O1#4−Cl1−O1#5	180.0
Symmetry codes: #1 −y, −z, −x; #2 y, z, x; #3 −x, −y, −z; #4 z, x, y; #5 −z, −x, −y.			

Table S2. Atomic coordinates and displacement parameters for **1**.

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
1 (223 K)				
C1	0.3167(4)	0.2500	0.6445(5)	0.0419(13)
C2	0.2542(5)	0.2500	0.5171(6)	0.070(2)
C3	0.1253(4)	0.2500	0.5389(6)	0.0563(16)
C4	0.0938(3)	0.0995(8)	0.6160(5)	0.0577(14)
C5	0.1582(3)	0.1017(5)	0.7435(3)	0.0467(11)
N1	0.2296(3)	0.2500	0.7491(4)	0.0351(11)
O1	0.2948(3)	0.2500	0.8646(3)	0.0562(14)
O2	0.0662(10)	0.1192(8)	0.2128(11)	0.184(4)
O3	0.2022(7)	0.2500	0.0917(8)	0.167(5)
O4	0.0248(7)	0.2500	0.0255(9)	0.258(9)
Cl1	0.08692(9)	0.2500	0.13300(12)	0.0405(8)
1 (353 K)				
C1	0.338(2)	0.338(2)	0.5000	0.249(16)
O1	0.0000	0.209(7)	0.0000	0.296(17)
Cl1	0.0000	0.0000	0.0000	0.139(8)

Table S3. Selected hydrogen bonds (Å, °) for **1**.

D–H···A	H···A	D···A	D–H···A
1 (273 K)			
O1–H1···O3#3	1.87	2.605(8)	147
Symmetry codes: #3 x, y, z+1.			