Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Order-Disorder Phase Transition Coupled with Torsion in Tri-*n*-ButylammoniumTrichloroacetate (TBAT)

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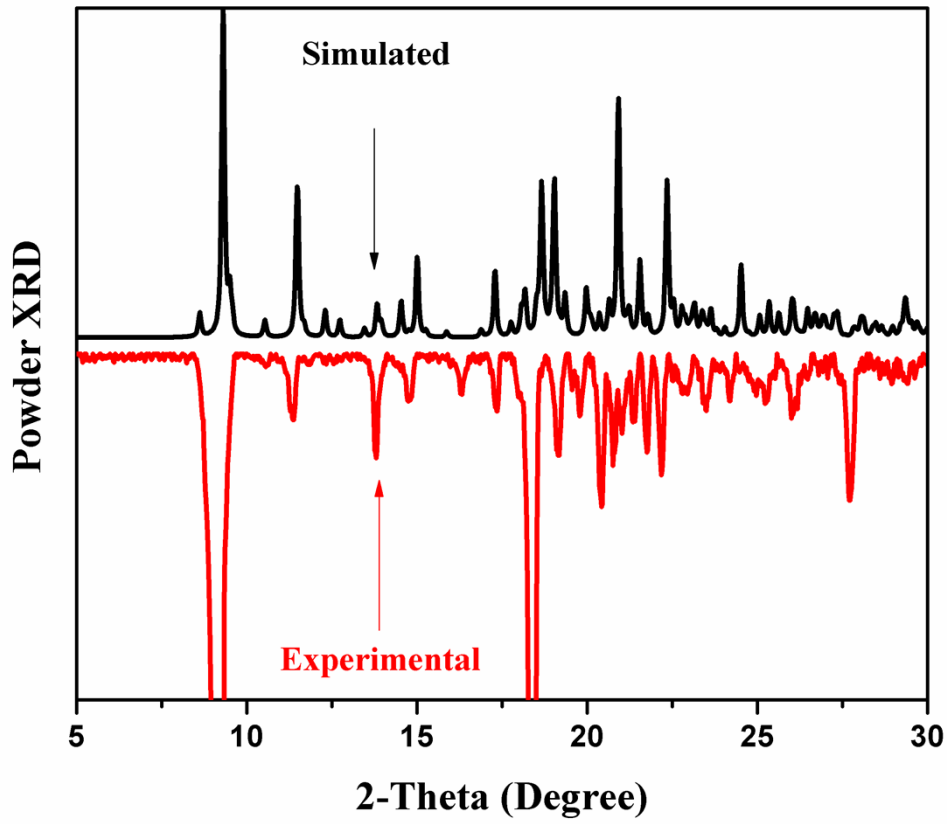

Figure S1. PXRD patterns of **TBAT.**

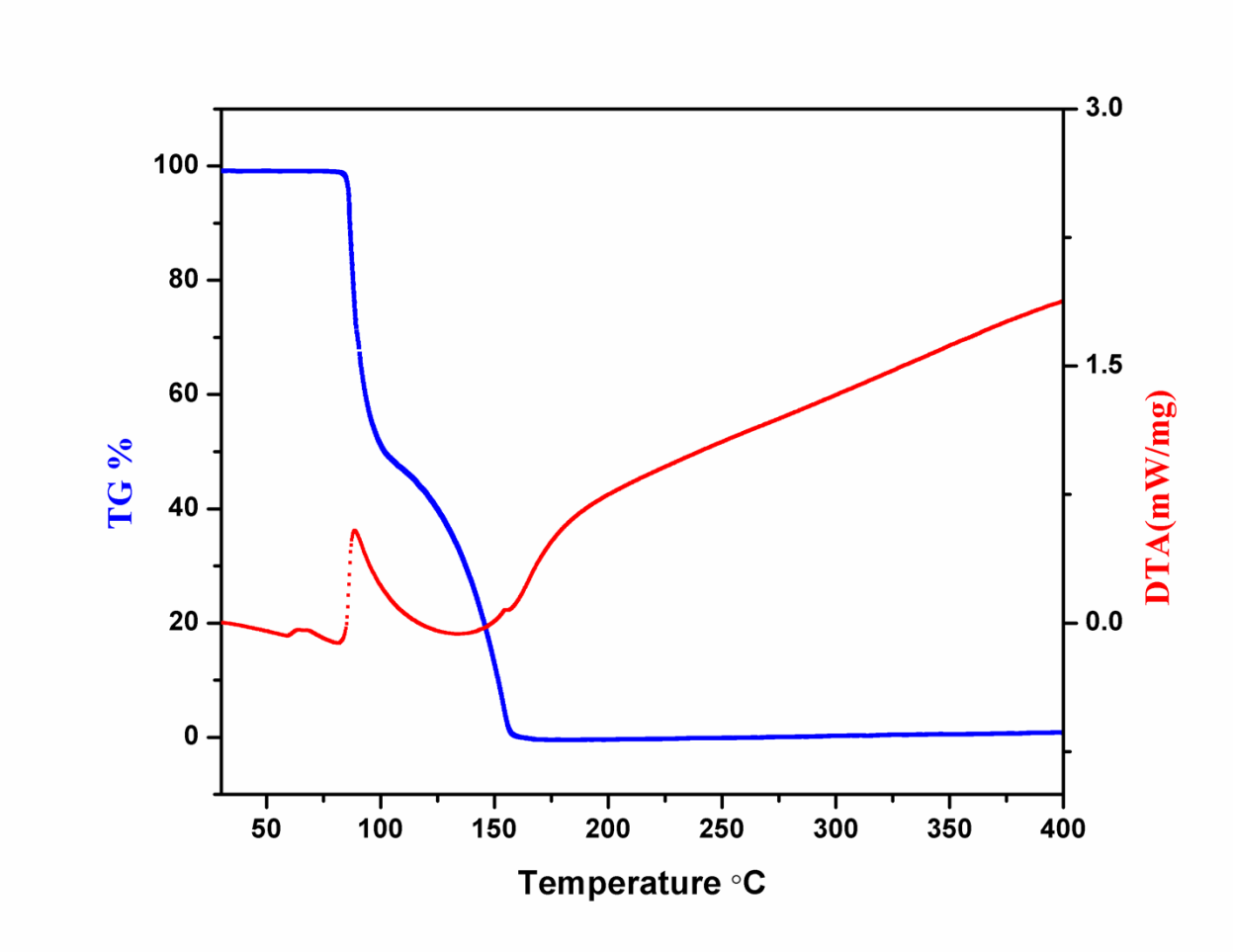

Figure S2. TG-DTA curves of **TBAT.**

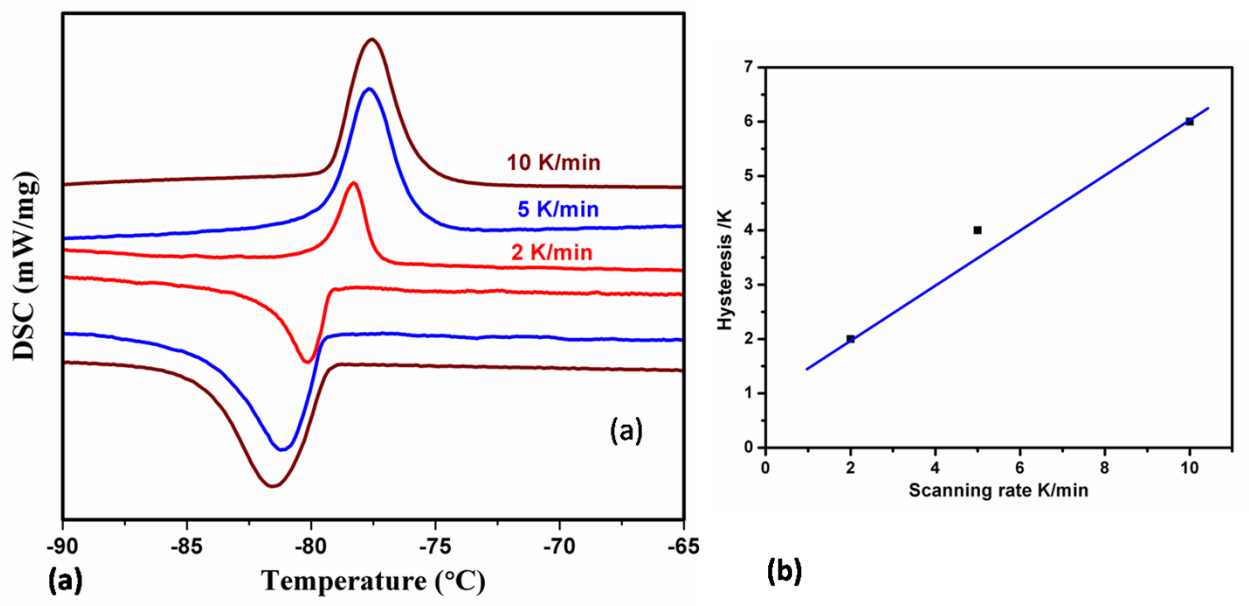

Figure S3. DSC curves of **TBAT** at (a) different scanning rates and (b) thermal hysteresis from the scans.

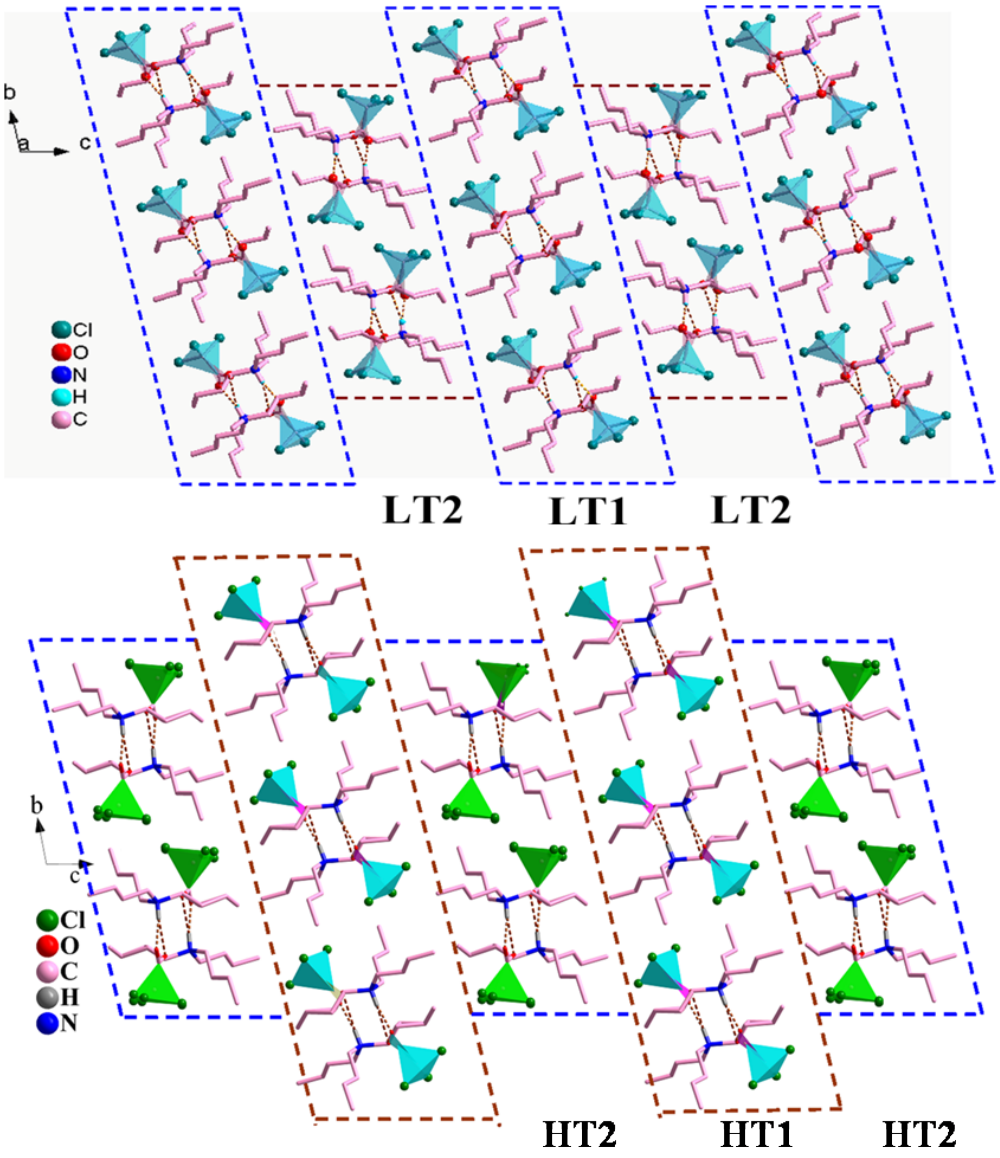

Figure S4. Unit cell packing diagrams viewed along the a-axis at (a) 100 and (b) 220 K of **TBAT**. The dotted lines stand for the hydrogen bonds.

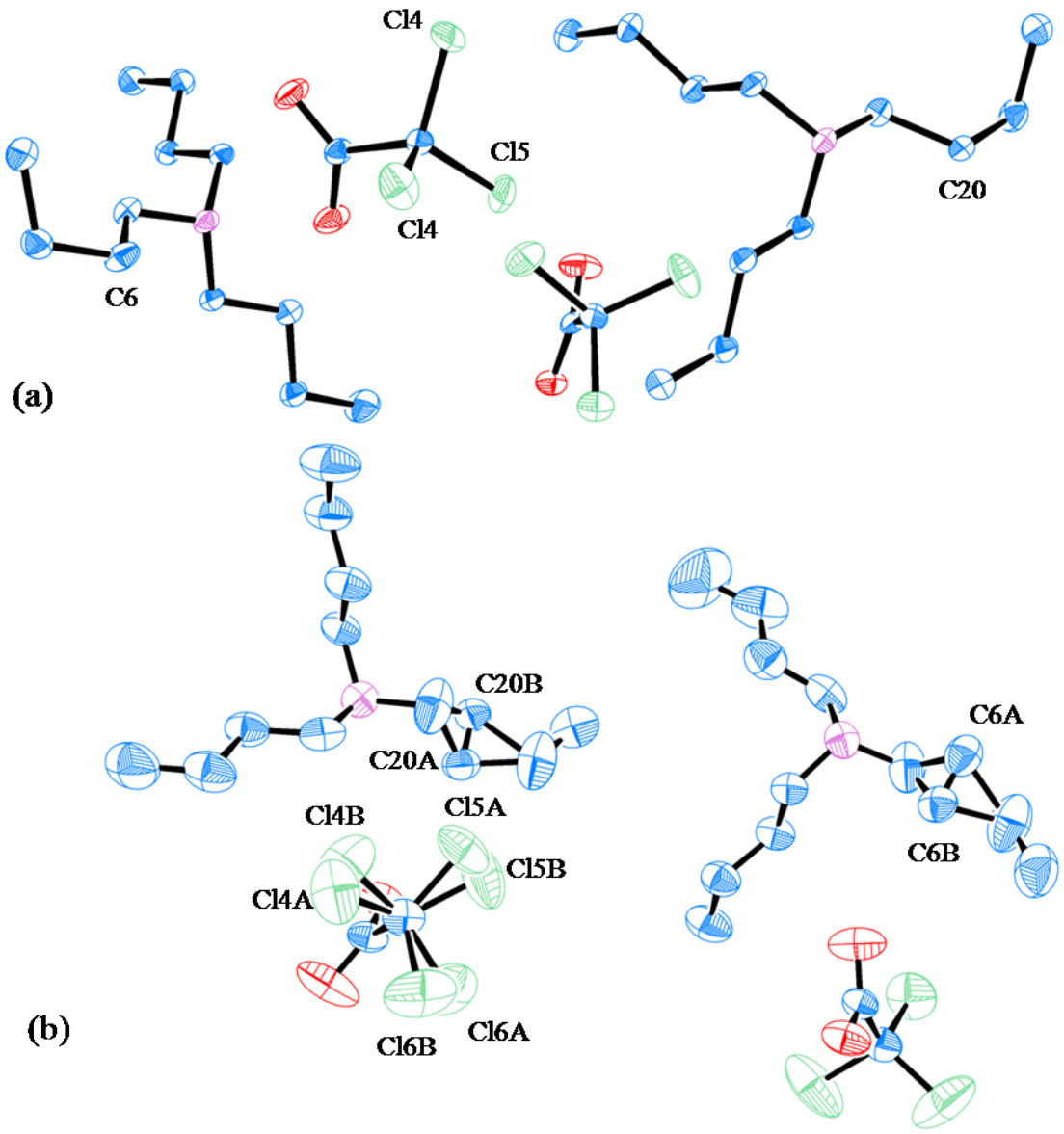

Figure S5. Thermal ellipsoidal view of **TBAT** at (a) 100 K and (b) at 220 K after splitting of appropriate atoms.

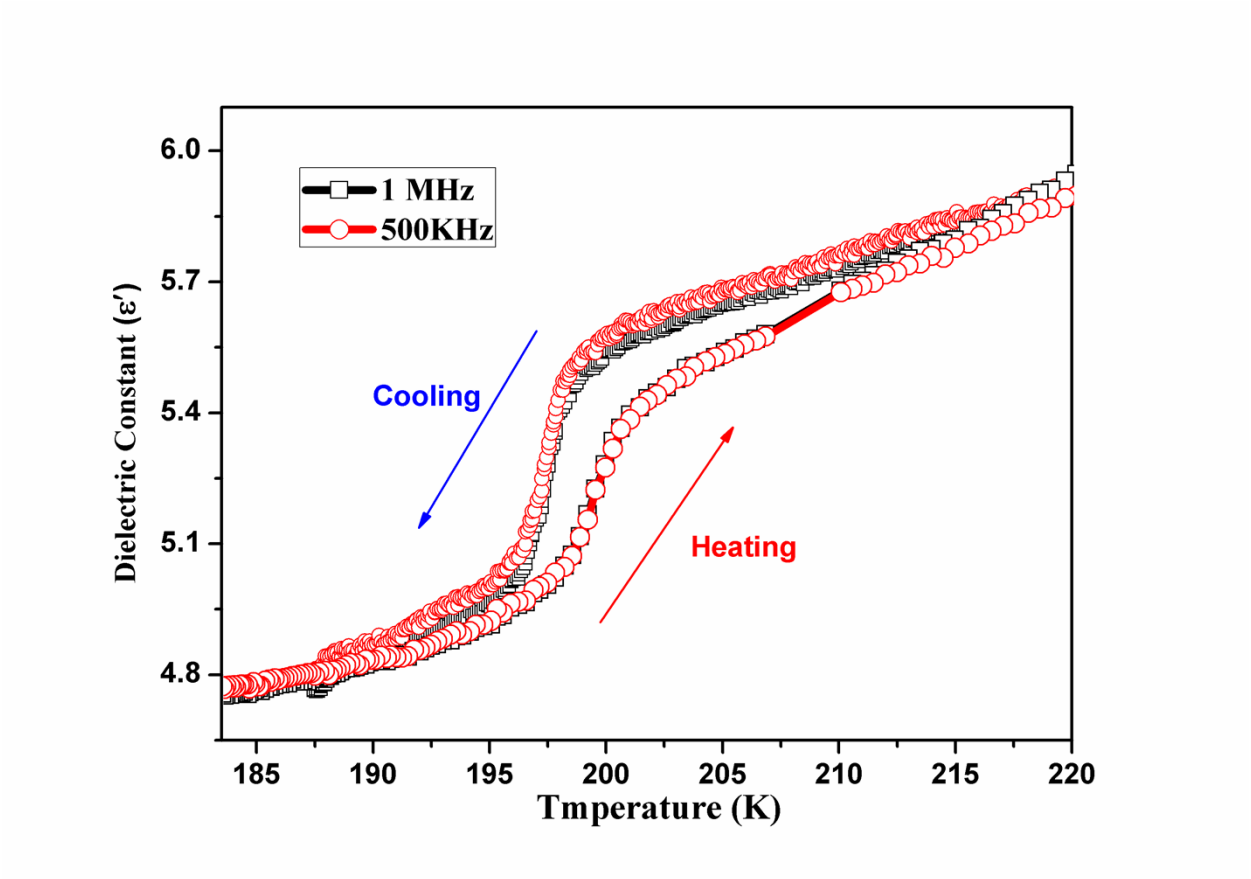

Figure S6. Temperature dependent cycle of dielectric constant of **TBAT** at 1 MHz and 500 KHz.

Table S1. Crystal Data and structure refinement details of **TBAT** at 100 and 220 K.

Sum formula	C14 H28 Cl3 N O2	C14 H28 Cl3 N O2
Formula weight	348.72	348.72
Temperature (K)	100	220
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	9.6337	9.6704
b/Å	10.7137	10.5407
c/Å	18.8281	19.7334
α/deg	98.742	98.677
β/deg	100.488	101.66
γ/deg	100.213	98.350
Volume (Å^3)	1846.15	1915.04
Z	2	2
D_{calcd}, g cm^{-1}	1.255	1.031
F(000)	744	744
Completeness (%)	98.3	99.8 %
Goodness-of-fit on F^2	1.038	1.056
R_1 (on F_o^2, $I>2\sigma(I)$)	0.0492	0.0652
wR_2 (on F_o^2, $I>2\sigma(I)$	0.1265	0.2573

Table S2. Hydrogen-bond geometry (Å, deg) at 100 and 220 K in **TBAT.**

100K	D—H	H···A	D···A	D—H···A
N1—H1...O1	0.93	1.79	2.716 (3)	170.5
N2—H2...O4	0.93	1.75	2.677 (3)	171.1
220K	D—H	H···A	D···A	D—H···A
N1—H1...O1	0.93	1.77	2.699 (3)	170.5
N2—H2...O4	0.93	1.81	2.738 (3)	171.1

Table S3. *Ueq* values of **TBAT** at 220 K.

Atoms	*U(equiv)*	Atoms	*U(equiv)*
C1	0.064	C15	0.052
C2	0.072	C16	0.062
C3	0.100	C17	0.072
C4	0.178	C18	0.098
C5	0.081	C19	0.093
C7	0.100	C21	0.102
C8	0.100	C22	0.117
C9	0.048	C23	0.057
C10	0.054	C24	0.062
C11	0.061	C25	0.082
C12	0.080	C26	0.101
C13	0.055	C27	0.051
C14	0.065	C28	0.061
N1	0.052	N2	0.050
O1	0.063	O3	0.061
O2	0.083	04	0.981
Cl1	0.133	Cl2	0.133
Cl3	0.093		