Supplementary Information

Dibenzylammonium trichloroacetate: An above-room-temperature order-disorder switchable dielectric material

Siyuan Zeng,[a] Zhihua Sun,[b] Chengmin Ji,[b] Shuquan Zhang,[b] Cheng Song,*[a] and Junhua Luo*[b]

[a]*College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang, Jiangxi 330022, PR China*

[b]*Key Laboratory of Optoelectronic Materials Chemistry and Physics, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, PR China*

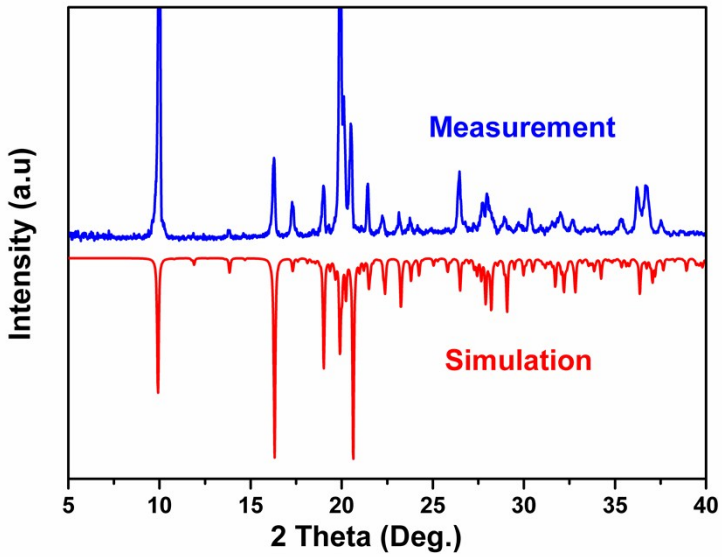

Figure S1. Experimental and calculated PXRD patterns of **1**.

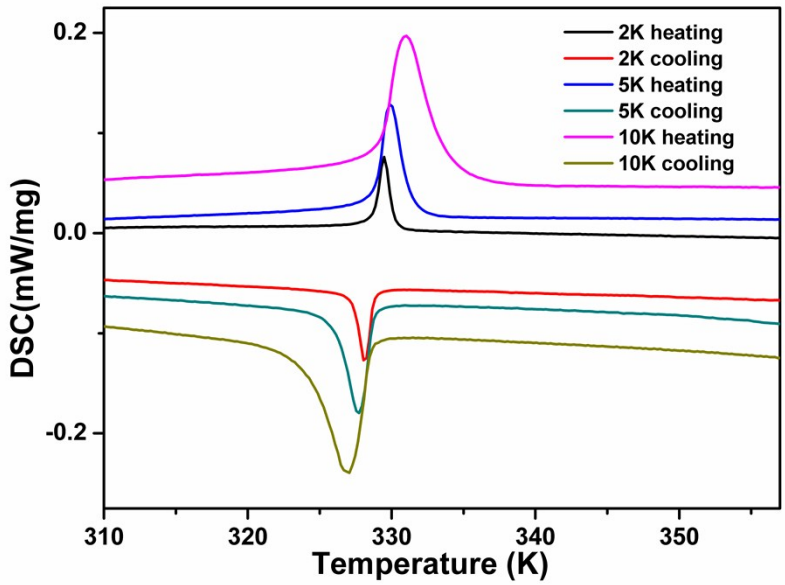

Figure S2. The DSC curves of **1** with different heating rate 10 K/min, 5 K/min, 2 K/min.

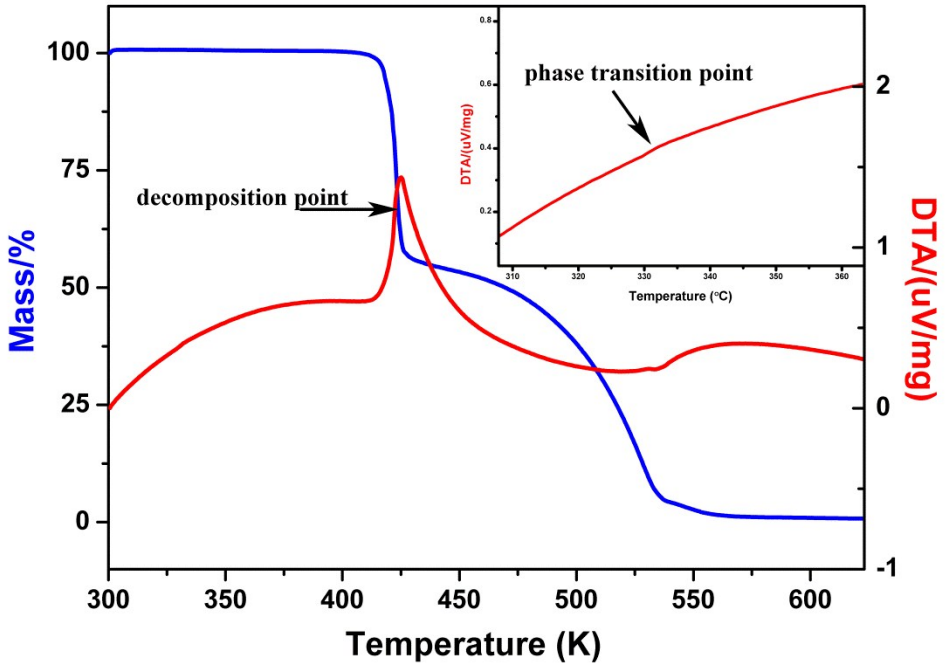

Figure S3. The TG/DTA curves of **1** with heating rate 10 K/min.

Table S1. Crystal data and structural refinement for **1** at different temperatures.

Temperature (K)	293K	310K	315K	320K
Radiation type	Mo	Cu	Cu	Cu
Empirical formula	$C_{24}H_{24}Cl_{4.5}N_{1.5}O_3$	$C_{24}H_{24}Cl_{4.5}N_{1.5}O_3$	$C_{24}H_{24}Cl_{4.5}N_{1.5}O_3$	$C_{24}H_{24}Cl_{4.5}N_{1.5}O_3$
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*P*nma	*P*nma	*P*nma	*P*nma
a (Å)	27.9771(10)	28.2608(3)	28.2714(3)	28.2869(4)
b (Å)	17.8261(7)	17.9257(3)	17.9408(2)	17.9428(3)
c (Å)	10.0751(3)	10.23480(10)	10.24460(10)	10.25130(10)
V (Å)^3	5024.7(3)	5184.89(11)	5196.18(9)	5203.01(12)
β (deg.)	90	90	90	90
Z	8	8	8	8
Calculated density (g cm^{-3})	1.430	1.385	1.382	1.381
Absorption coefficient (mm^{-1})	0.552	4.835	4.831	4.832
F (000)	2232	2230	2231	2232
Theta range for data	2.71 to 26.37	3.98 to 66.60	3.98 to 66.59	3.12 to 66.58
Index ranges	-23≤h≤34 -22≤k≤21 -12≤l≤12	-33≤h≤21 -21≤k≤20 -8≤l≤12	-27≤h≤33 -21≤k≤21 -12≤l≤12	-33≤h≤21 -21≤k≤19 -12≤l≤11
Reflections collected	16412 / 5280	14382 / 4693	27392 / 4744	12575 / 4755
GOF	1.024	1.065	1.060	1.077
R_1, wR_2 [$I>2\sigma$(I)]	0.0400, 0.0932	0.0743, 0.2093	0.0775, 0.2158	0.0850, 0.2402
R_1, wR_2 [all data]	0.0565, 0.1030	0.0894, 0.2332	0.0886, 0.2301	0.1013, 0.2619

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (Å×10^3) for **1** at 293K. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl1	7806 (3)	4457	3058 (7)	44.5 (2)
Cl2	10248 (3)	5888 (4)	3423 (7)	72.8 (2)
O1	8062 (7)	4457	5934 (2)	44.9 (5)
O2	10275 (7)	4457	6076 (18)	40.7 (5)
N1	18426 (7)	13370	1279 (2)	28.9 (5)
C23	9352 (9)	4457	3914 (3)	28.3 (6)
C22	9205 (9)	4457	5477 (3)	27.9 (6)
C2	18457 (7)	10887 (12)	1339 (2)	35.0 (5)
C3	17571 (7)	10291 (13)	450 (2)	40.3 (5)
C1	19203 (7)	12133 (12)	974 (2)	39.6 (5)
C5	17186 (8)	8500 (13)	1982 (2)	48.1 (6)
C7	18682 (8)	10278 (12)	2560 (2)	42.1 (5)
C4	16945 (8)	9104 (13)	773 (2)	45.6 (5)
C6	18046 (9)	9092 (13)	2878 (2)	47.8 (6)

Table S3. Selected bond lengths (Å) and angles (°) for N-IPBADC at 293K.

Cl1—C23	1.768 (3)	C7—C6	1.382 (3)	C23—C22	1.569 (4)
Cl2—C23	1.7589 (16)	C2—C7	1.383 (3)	N1—C1	1.492 (2)
O1—C22	1.232 (3)	C2—C3	1.389 (3)	C5—C4	1.373 (3)
O2—C22	1.227 (3)	C2—C1	1.498 (3)	C5—C6	1.376 (3)
C3—C4	1.380 (3)				

C4—C3—C2	120.6 (2)	C5—C6—C7	120.5 (2)
C1—N1—C1^{ii}	112.0 (2)	N1—C1—C2	112.38 (16)
O2—C22—O1	128.9 (3)	C4—C5—C6	119.6 (2)
O2—C22—C23	113.9 (2)	C6—C7—C2	120.4 (2)
O1—C22—C23	117.2 (2)	C7—C2—C3	118.7 (2)
C5—C4—C3	120.3 (2)	C7—C2—C1	120.02 (19)
C22—C23—Cl2^{i}	109.02 (11)	C3—C2—C1	121.28 (19)
Cl2—C23—Cl2^{i}	108.98 (15)	Cl2—C23—Cl1	108.08 (10)
C22—C23—Cl1	113.59 (18)	Cl2^{i}—C23—Cl1	108.08 (10)
C22—C23—Cl2	109.02 (11)		

Table S4. Equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the chlorine of **1** at different temperatures. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	U(eq)			
	293 K	310 K	315 K	320 K
Cl(1)	44.5(2)	147.8(13)	162(12)	200(2)
Cl(2)	72.8(2)	127.2(2)	144.8(16)	260(2)