Supplementary Information

Switchable Dielectric Behaviour Associated with Above Room-Temperature Phase Transition in N-Isopropylbenzylammonium Dichloroacetate (N-IPBADC)

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Table S1. Crystal data and structural refinement for N-IPBADC at different temperatures.

Temperature (K)	293	323	343	356	358
Empirical formula	$C_{12}H_{17}Cl_2NO_2$	$C_{12}H_{17}Cl_2NO_2$	$C_{12}H_{17}Cl_2NO_2$	$C_{12}H_{17}Cl_2NO_2$	$C_{12}H_{17}Cl_2NO_2$
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	9.700(8)	9.7598(3)	9.7856(5)	9.7987(8)	9.8256(9)
b (Å)	8.569(6)	8.5995(2)	8.6119(3)	8.6320(4)	8.6329(5)
c (Å)	17.378(14)	17.5609(6)	17.6992(11)	17.6834(11)	17.8841(19)
V (Å^3)	1389.7(18)	1416.03(7)	1429.77(13)	1444.08(16)	1450.2(2)
β (deg.)	105.825(13)	106.105(4)	106.549 (5)	106.919(7)	107.061 (8)
Z	4	4	4	4	4
Calculated density (g cm^{-3})	1.329	1.305	1.292	1.280	1.274
Absorption coefficient (mm^{-1})	0.457	0.449	0.445	0.440	0.438
F(000)	584.0	584.0	584.0	584.0	584.0
Theta range for data	2.67 to 27.50	3.21 to 26.37	3.20 to 26.37	3.19 to 26.37	3.19 to 26.37

collection					
Index ranges	-12≤h≤12, -10≤k≤11, -22≤l≤22	-12≤h≤12, -10≤k≤10, -21≤l≤21	-12≤h≤12, -10≤k≤10, -20≤l≤22	-12≤h≤12, -10≤k≤10, -22≤l≤20	-12≤h≤12, -10≤k≤10, -21≤l≤22
Reflections collected	10400 / 3168	8874 / 2886	8983 / 2922	9116 / 2957	8979 / 2965
GOF	1.103	1.073	1.088	1.102	1.031
R_1, wR_2 [$I>2\sigma(I)$]	0.0560, 0.1437	0.0688, 0.1916	0.0824, 0.2368	0.0889, 0.2759	0.0475, 0.1230
R_1, wR_2 [all data]	0.0702, 0.1604	0.0879, 0.2137	0.1060, 0.2664	0.1167, 0.3091	0.0810, 0.1526

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2\times10^3$) for N-IPBADC at 293K. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(2)	1260(1)	3362(1)	102(1)	78(1)
Cl(1)	1899(1)	113(1)	-73(1)	77(1)
N(1)	-4473(2)	2413(2)	-1970(1)	41(1)
O(2)	3734(2)	3144(2)	1472(1)	69(1)
C(12)	3376(2)	1827(3)	1230(1)	46(1)
O(1)	4023(2)	615(2)	1467(1)	72(1)
C(6)	-2254(2)	2383(3)	-2404(1)	45(1)
C(7)	-3146(3)	3285(3)	-1972(2)	57(1)
C(11)	1902(3)	1633(3)	615(1)	51(1)
C(1)	-1107(3)	1509(3)	-1977(2)	54(1)
C(8)	-5420(3)	3203(3)	-1531(2)	53(1)
C(2)	-280(3)	685(3)	-2364(2)	65(1)
C(5)	-2553(3)	2422(3)	-3227(2)	57(1)
C(10)	-6817(3)	2324(4)	-1711(2)	74(1)
C(3)	-578(3)	732(4)	-3178(2)	67(1)
C(4)	-1709(3)	1604(4)	-3612(2)	67(1)
C(9)	-4693(4)	3287(4)	-657(2)	83(1)

Table 3. Selected bond lengths (Å) and angles (°) for N-IPBADC at 293K.

Cl(2)-C(11)	1.753(3)	C(12)-O(1)	1.225(3)	C(1)-C(2)	1.374(4)
Cl(1)-C(11)	1.767(3)	C(12)-C(11)	1.542(3)	C(8)-C(9)	1.492(4)
N(1)-C(7)	1.489(3)	C(6)-C(1)	1.378(3)	C(8)-C(10)	1.506(4)
N(1)-C(8)	1.506(3)	C(6)-C(5)	1.380(3)	C(2)-C(3)	1.365(4)
O(2)-C(12)	1.222(3)	C(6)-C(7)	1.503(3)	C(5)-C(4)	1.381(4)
C(3)-C(4)	1.371(4)				
C(7)-N(1)-C(8)	115.06(18)	O(2)-C(12)-O(1)	126.6(2)	O(2)-C(12)-C(11)	117.4(2)
O(1)-C(12)-C(11)	115.8(2)	C(1)-C(6)-C(5)	118.8(2)	C(1)-C(6)-C(7)	120.1(2)
C(5)-C(6)-C(7)	121.2(2)	N(1)-C(7)-C(6)	111.02(19)	C(12)-C(11)-Cl(2)	113.28(16)

C(12)-C(11)-Cl(1)	112.22(17)	Cl(2)-C(11)-Cl(1)	110.09(14)	C(2)-C(1)-C(6)	120.6(2)
C(9)-C(8)-N(1)	110.7(2)	C(9)-C(8)-C(10)	112.6(2)	N(1)-C(8)-C(10)	108.0(2)
C(3)-C(2)-C(1)	120.3(2)	C(6)-C(5)-C(4)	120.4(2)	C(2)-C(3)-C(4)	119.9(3)
C(3)-C(4)-C(5)	120.1(3)				

Table 4. Equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the chlorine of N-IPBADC at different temperatures. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	U(eq)			
	293 K	323 K	343 K	356 K
Cl(1)	77(1)	92(1)	108(1)	129(1)
Cl(2)	78(1)	93(1)	110(1)	126(1)

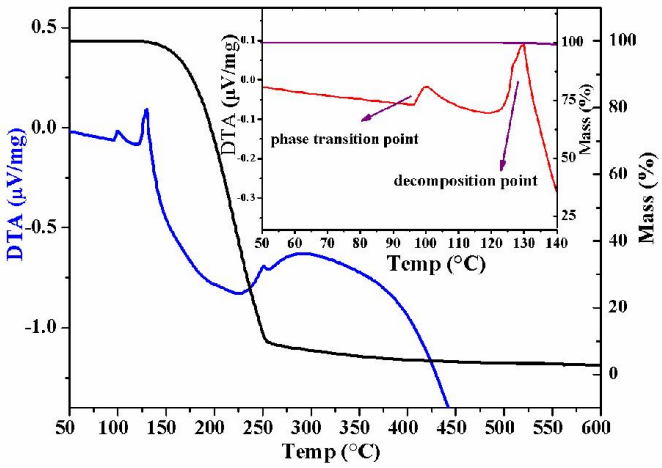

Figure S1. The TG/DTA curves of N-IPBADC with heating rate 5 °C/min.

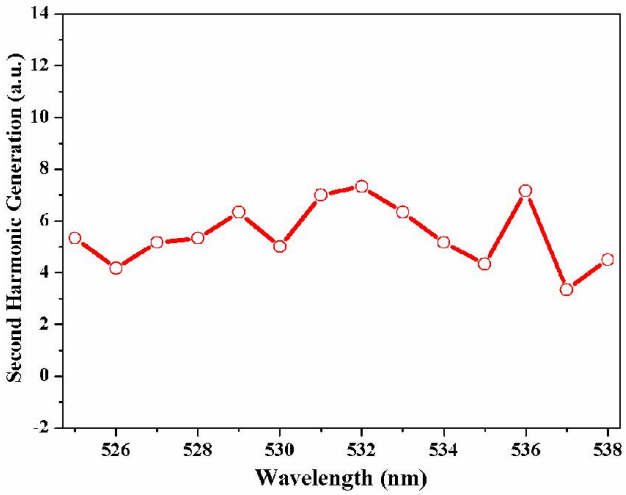

Figure S2. The SHG signals of N-IPBADC at room temperature with 1064 nm irritation.

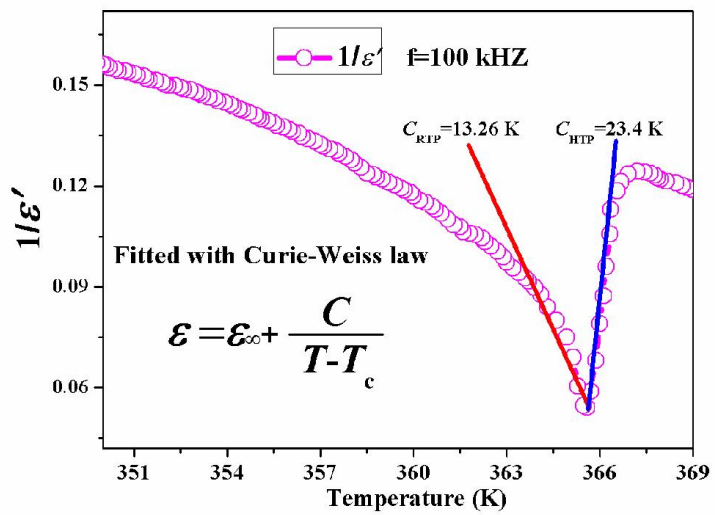

Figure S3. The Curie-Weiss law ftting of the dielectric constants at a frequency of 100 KHz in the interval of phase transition.

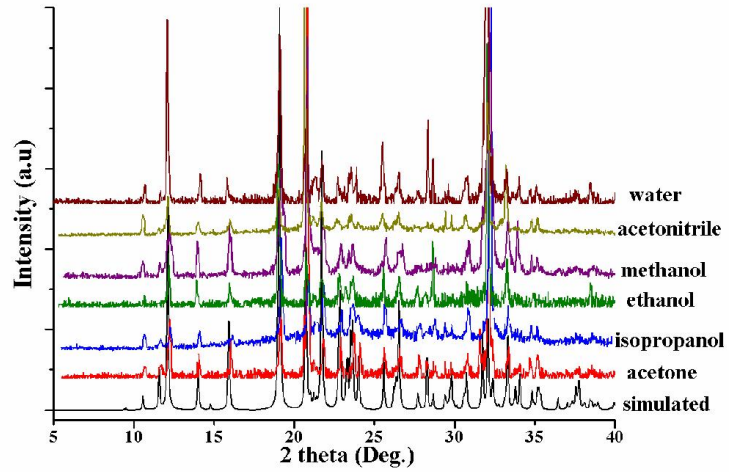

Figure S4. PXRD patterns of N-IPBADC crystallized in various solvents.