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

Supplementary Information

N-Isopropylbenzylammonium Tetrafluoroborate: An Organic Dielectric Relaxor with Tunable Transition between High and Low Dielectric States

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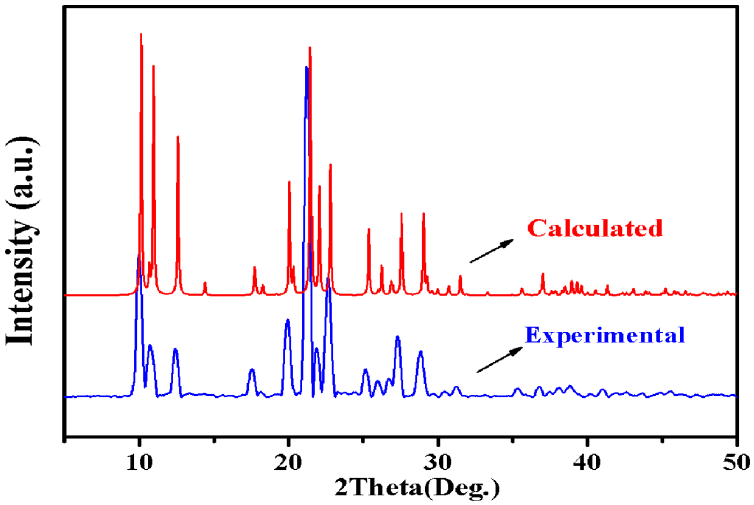

Figure S1. Simulated and experimental XRD powder patterns for compounds 1.

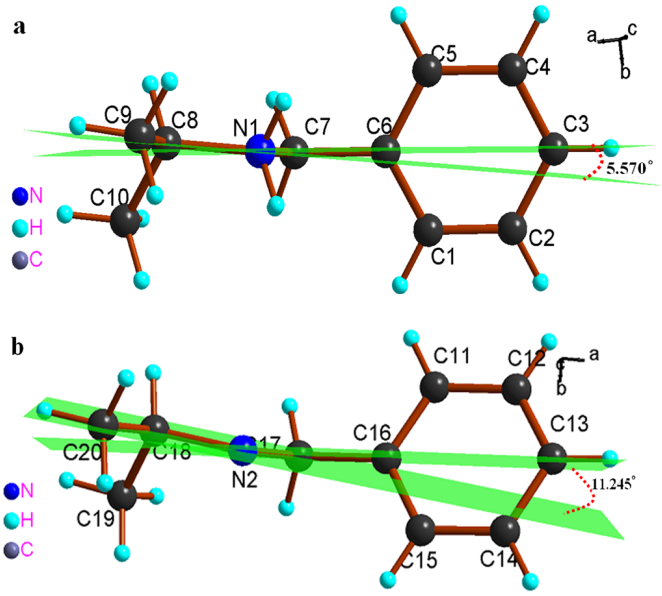

Figure S2. The dihedral angle of the different configurational N-MBA cations in low temperature phase: (a)LTPa and (b)LTPb.

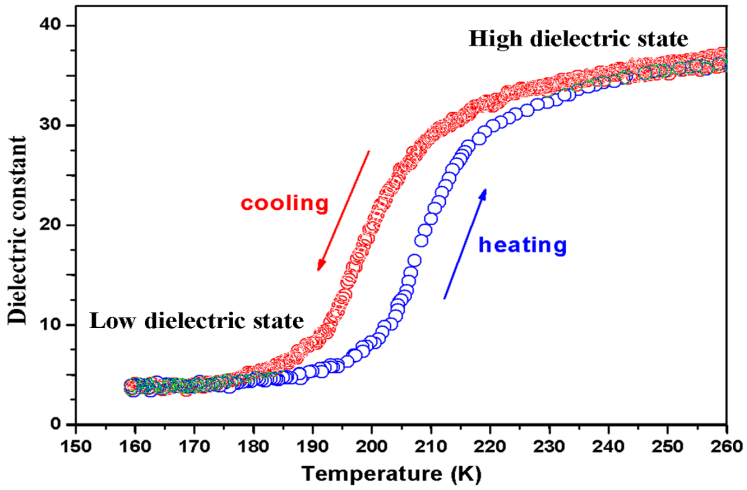

Figure S3. Dielectric constant measured in the cooling and heating cycle at 100 KHz.

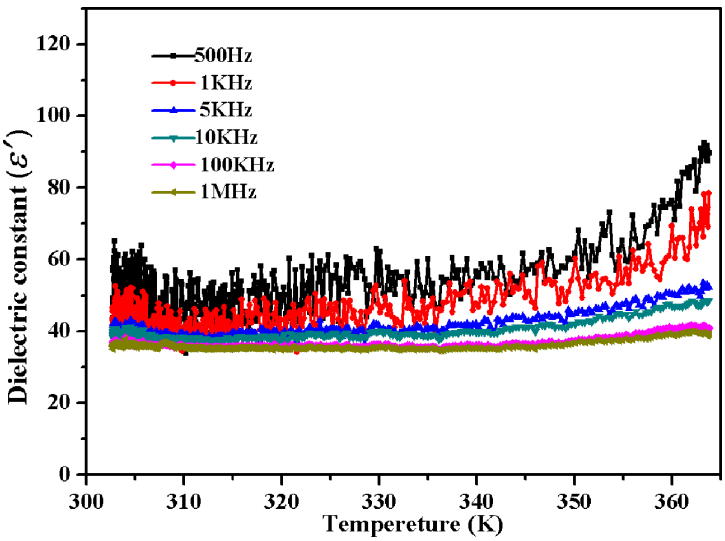

Figure S4. Dielectric constant measured at the high temperature .

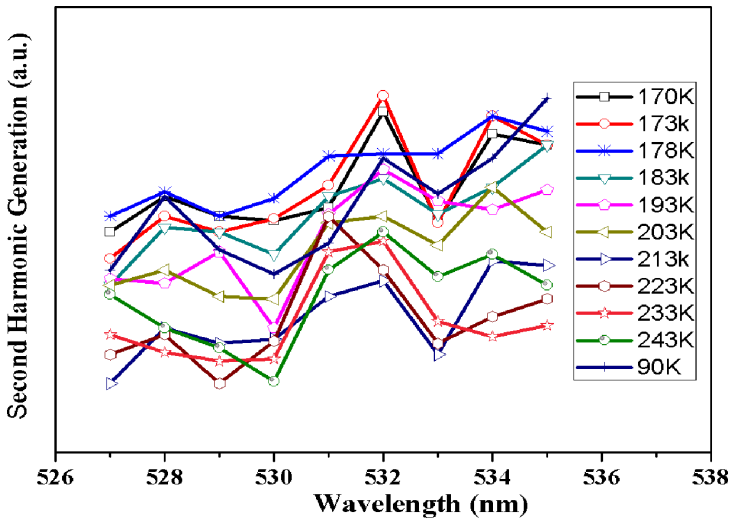

Figure S5. The second-order nonlinear optical experiment at 532 nm at different temperature.

Table S1. Crystal data and structural refinement for compound **1**

Empirical formula	$C_{10}H_{16}BF_4N$	$C_{10}H_{16}BF_4N$
Formula weight	244.26	244.26
Temperature/K	293(2)	100(2)
Radiation	Mo-Kα (0.71073 Å)	Mo-Kα (0.71073 Å)
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/m	*C*2/c
a/Å	18.493(4)	19.550(4)
b/Å	7.7954(16)	7.7410(15)
c/Å	10.016(2)	32.466(7)
α/deg	90	90
β/deg	119.35(3)	95.61(3)
γ/deg	90	90
Volume/ Å^3	1258.6(4)	4889.8(17)
Z	4	16
Calculated density/g cm^{-3}	1.262	1.288
Absorption coefficient/mm^{-1}	0.114	0.117
F(000)	504.0	1984.0
Crystal size/mm	0.33×0.24×0.16	0.33×0.24×0.16
Limiting indices	-18<=h<=24, -9<=k<=10, -13<=l<=12	-24<=h<=25, -10<=k<=8, -41<=l<=33
Reflections collected / unique	3963 / 1547[*R*(int) = 0.0227]	13402/ 5434 [R(int) = 0.0434]
GOF	1.044	1.024
R_1, wR_2 [$I>2\sigma(I)$]	0.0939/0.3083	0.0800/0.2094
R_1, wR_2 (all data)	0.1459/0.3382	0.0964/0.2236

Table 2. Selected bond lengths (Å) and angles (°) for compound **1** (293K)

bond lengths	(Å)	bond lengths	(Å)	bond lengths	(Å)
N(1)-C(5)	1.484(5)	F(2)-B(1)	1.358(4)	B(1)-F(3)	1.336(7)
N(1)-C(6)	1.483(5)	C(6)-C(7)#1	1.374(9)	B(1)-F(2)#1	1.358(4)
C(1)-C(2)	1.358(6)	C(6)-C(7)	1.374(9)	C(2)-C(3)	1.388(7)
C(1)-C(2)#1	1.358(6)	C(6)-C(8)	1.486(7)	C(7)-C(7)#1	1.230(19)
C(1)-C(5)	1.499(7)	B(1)-F(1)	1.287(7)	C(4)-C(3)#1	1.349(9)
				C(4)-C(3)	1.349(9)

bond angles	(°)	bond angles	(°)	bond angles	(°)
C(5)-N(1)-C(6)	117.2(3)	F(1)-B(1)-F(2)#1	112.0(4)	C(7)-C(6)-N(1)	120.3(5)
C(2)-C(1)-C(2)#1	120.4(6)	F(3)-B(1)-F(2)#1	110.4(4)	C(8)-C(6)-N(1)	109.4(4)
C(2)-C(1)-C(5)	119.8(3)	F(1)-B(1)-F(2)	112.0(4)	F(1)-B(1)-F(3)	106.7(5)
C(2)#1-C(1)-C(5)	119.8(3)	F(3)-B(1)-F(2)	110.4(4)	C(7)-C(6)-C(8)	122.0(5)
N(1)-C(5)-C(1)	112.5(3)	F(2)#1-B(1)-F(2)	105.4(4)	C(7)#1-C(6)-N(1)	120.3(5)
C(7)#1-C(6)-C(7)	53.2(8)	C(1)-C(2)-C(3)	120.2(6)	C(3)#1-C(4)-C(3)	123.4(10)
C(7)#1-C(6)-C(8)	122.0(5)	C(7)#1-C(7)-C(6)	63.4(4)	C(4)-C(3)-C(2)	117.9(8)

Symmetry transformations used to generate equivalent atoms: #1 x,-y,z

Table 3. Selected bond lengths (Å) and angles (°) of 1 in low temperature phase.

bond lengths	(Å)	bond lengths	(Å)	bond lengths	(Å)
F(7)-B(2)	1.410(4)	C(18)-C(19)	1.514(5)	C(14)-C(15)	1.378(7)
N(2)-C(17)	1.505(4)	C(17)-C(11)	1.508(4)	C(12)-C(13)	1.386(5)
N(2)-C(18)	1.513(3)	C(11)-C(12)	1.386(5)	C(16)-C(15)	1.394(5)
F(5)-B(2)	1.373(4)	C(11)-C(16)	1.388(5)	F(1)-B(1)	1.400(4)
F(6)-B(2)	1.380(4)	F(8)-B(2)	1.365(4)	N(1)-C(8)	1.505(4)
C(18)-C(20)	1.501(4)	C(14)-C(13)	1.366(6)	C(8)-C(9)	1.507(4)
N(1)-C(7)	1.499(4)	C(2)-C(3)	1.391(6)	C(3)-C(4)	1.371(15)
C(8)-C(10)	1.523(5)	C(1)-C(2)	1.364(7)	C(6)-C(5)	1.407(8)
F(2)-B(1)	1.383(5)	C(1)-C(6)	1.395(6)	C(4)-C(5)	1.330(15)
C(7)-C(1)	1.502(5)	F(4)-B(1)	1.314(5)	F(3)-B(1)	1.369(5)

bond angles	(°)	bond angles	(°)	bond angles	(°)
C(17)-N(2)-C(18)	117.9(8)	F(6)-B(2)-F(7)	107.0(3)	C(2)-C(1)-C(7)	121.2(4)
C(20)-C(18)-N(2)	111.9(2)	C(13)-C(14)-C(15)	120.3(3)	C(1)-C(2)-C(3)	120.5(6)
C(20)-C(18)-C(19)	112.9(3)	F(1)-B(1)-F(2)	120.3(3)	F(4)-B(1)-F(3)	107.6(4)
N(2)-C(18)-C(19)	107.3(2)	C(11)-C(12)-C(13	120.3(4)	F(4)-B(1)-F(2)	112.4(4)
N(2)-C(17)-C(11)	111.6(2)	C(11)-C(16)-C(15)	119.7(4)	F(3)-B(1)-F(2)	108.8(4)
C(12)-C(11)-C(16)	119.4(3)	C(14)-C(15)-C(16)	120.1(4)	F(4)-B(1)-F(1)	110.9(4)
C(12)-C(11)-C(17)	120.5(3)	C(14)-C(13)-C(12)	120.2(4)	F(3)-B(1)-F(1)	109.7(3)
C(16)-C(11)-C(17)	120.0(3)	C(7)-N(1)-C(8)	114.6(2)	F(2)-B(1)-F(1)	107.4(3)
F(8)-B(2)-F(5)	109.6(3)	N(1)-C(8)-C(9)	111.6(2)	C(4)-C(3)-C(2)	120.0(8)
F(8)-B(2)-F(6)	111.6(3)	N(1)-C(8)-C(10)	107.4(3)	C(1)-C(6)-C(5)	117.8(7)
F(5)-B(2)-F(6)	109.8(3)	C(9)-C(8)-C(10)	112.5(3)	C(5)-C(4)-C(3)	119.7(6)
F(8)-B(2)-F(7)	108.6(3)	N(1)-C(7)-C(1)	111.8(3)	C(4)-C(5)-C(6)	122.3(8)
F(5)-B(2)-F(7)	110.2(3)	C(2)-C(1)-C(6)	119.6(4)		

Table 4. Torsion angle of 1 in room temperature phase.

C(6)-N(1)-C(5)-C(1)	180.000(1)
C(2)-C(1)-C(5)-N(1)	-91.8(4)
C(2)#1-C(1)-C(5)-N(1)	91.8(4)
C(5)-N(1)-C(6)-C(7)#1	31.2(5)
C(5)-N(1)-C(6)-C(7)	-31.2(5)
C(5)-N(1)-C(6)-C(8)	180.000(1)
C(2)#1-C(1)-C(2)-C(3)	-0.7(9)
C(5)-C(1)-C(2)-C(3)	-177.1(5)
C(8)-C(6)-C(7)-C(7)#1	-108.2(4)
N(1)-C(6)-C(7)-C(7)#1	107.0(4)
C(3)#1-C(4)-C(3)-C(2)	2.7(15)
C(1)-C(2)-C(3)-C(4)	-0.9(9)

Symmetry transformations used to generate equivalent atoms: #1 x,-y,z

Table 5. Torsion angle of 1 in low temperature phase.

C8-N1-C7-C6	-174.4(2)
N1-C7-C6-C5	80.1(3)
N1-C7-C6-C1	-102.4(3)
C7-N1-C8-C10	-58.8(3)
C7-N1-C8-C9	176.2(2)
C5-C6-C1-C2	-0.4(4)
C7-C6-C1-C2	-177.9(2)
C1-C6-C5-C4	0.6(4)
C7-C6-C5-C4	178.1(2)
C2-C3-C4-C5	-0.7(5)
C6-C5-C4-C3	-0.1(5)
C4-C3-C2-C1	0.9(5)
C6-C1-C2-C3	-0.4(4)
C17-N2-C18-C19	-57.2(3)
C17-N2-C18-C20	178.9(2)
C18-N2-C17-C16	-168.8(2)
N2-C17-C16-C15	-72.0(3)
N2-C17-C16-C11	110.6(3)
C11-C16-C15-C14	-0.8(5)
C17-C16-C15-C14	-178.1(3)
C16-C15-C14-C13	1.1(6)
C15-C16-C11-C12	-0.6(5)
C17 -C16-C11-C12	176.8(3)
C16-C11-C12-C13	1.8(6)
C11 -C12-C13-C14	-1.5(7)
C15-C14-C13-C12	0.1(7)