

Supporting Information

Two-step synthesized method strategy of long-range ordered and relaxor ferroelectrics achieves excellent electrical performance and thermal stability in BF-BT based Ceramics

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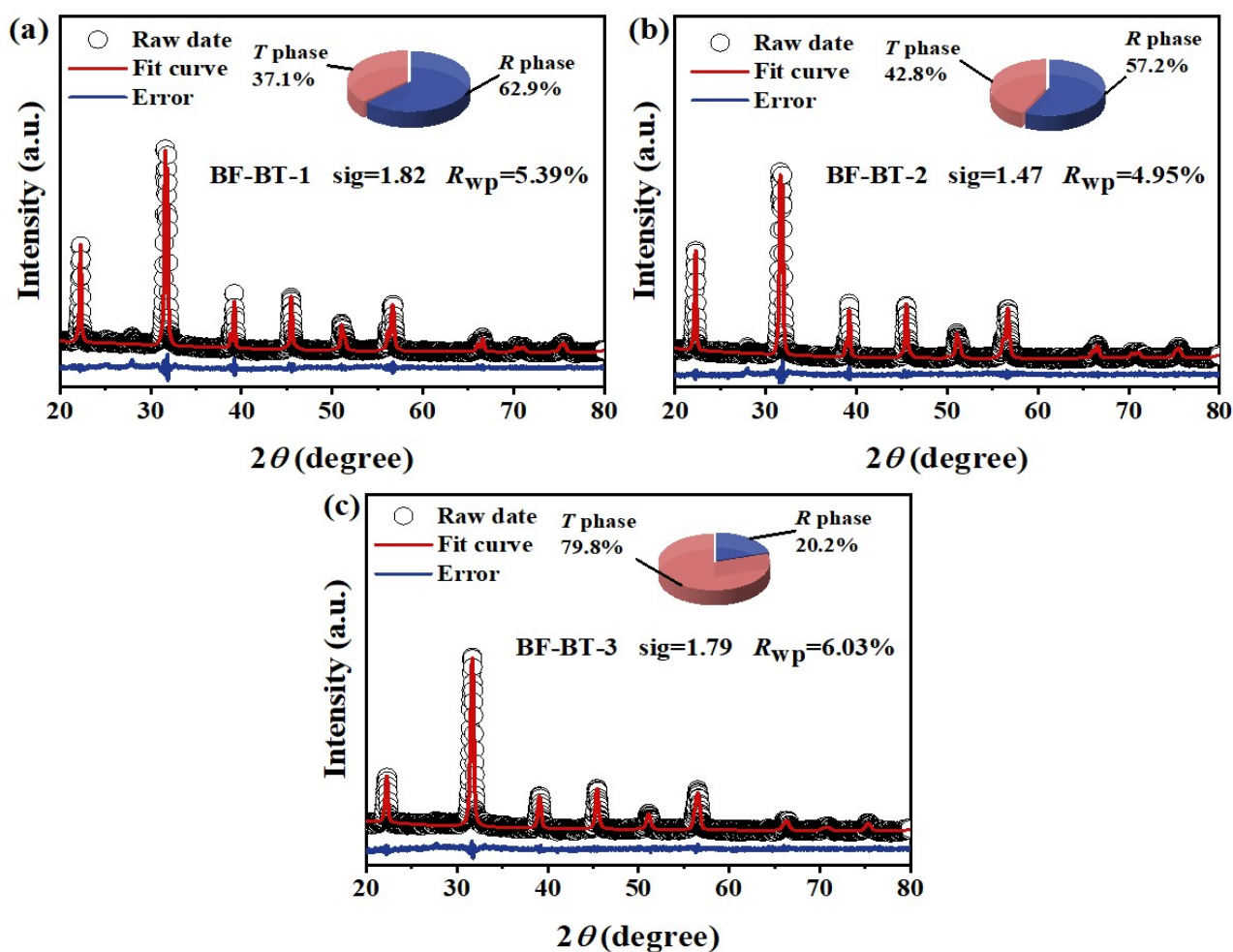


Fig. S1. (a-c) Rietveld refinement of crystal structures of BF-BT-1, BF-BT-2, BF-BT-3.

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Table S1 Results of crystal parameters after structural refinement

Parameters	BF-BT-1		BF-BT-2		BF-BT-3		BF-BT-4	
sig	1.82		1.47		1.79		1.67	
R_w (%)	5.39		4.95		6.03		5.18	
phase content (%)	<i>R</i> phase (62.9)	<i>T</i> phase (37.1)	<i>R</i> phase (57.2)	<i>T</i> phase (42.8)	<i>R</i> phase (20.2)	<i>T</i> phase (79.8)	<i>R</i> phase (49.4)	<i>T</i> phase (50.6)
Space group	<i>R3c</i>	<i>P4mm</i>	<i>R3c</i>	<i>P4mm</i>	<i>R3c</i>	<i>P4mm</i>	<i>R3c</i>	<i>P4mm</i>
<i>a</i> (Å)	5.6151	4.0021	5.6165	3.9810	5.6258	3.9898	5.6213	3.9878
<i>b</i> (Å)	5.6151	4.0021	5.6165	3.9810	5.6258	3.9898	5.6213	3.9878
<i>c</i> (Å)	13.9110	3.9773	13.9071	4.0347	13.8005	4.0176	13.9062	4.0131
Volume (Å ³)	379.84	63.70	379.93	63.94	378.26	63.95	380.55	63.8185
$\alpha = \beta = \gamma$ (°)	89.387	90	89.406	90	89.921	90	89.466	90

Table S2 Atomic positions after structural refinement

Chemical Element	BF-BT-1			BF-BT-2			BF-BT-3			BF-BT-4		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
-	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
Bi	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Fe	0.0000	0.0000	0.2417	0.0000	0.0000	0.2212	0.0000	0.0000	0.2212	0.0000	0.0000	0.2212
O (<i>R</i>)	0.5104	0.0278	0.8949	0.4430	0.0120	0.9543	0.4430	0.0120	0.9543	0.4430	0.0120	0.9543
Ba	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ti	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000	0.4997	0.5000	0.4999	0.5000	0.5000	0.5000
O ₁ (<i>T</i>)	0.5000	0.5000	0.0000	0.5003	0.5001	0.0003	0.5004	0.5003	0.0001	0.5001	0.5001	0.0001
O ₂ (<i>T</i>)	0.5000	0.0000	0.5000	0.5003	0.0004	0.5004	0.5005	0.0003	0.5004	0.5005	0.0000	0.5003

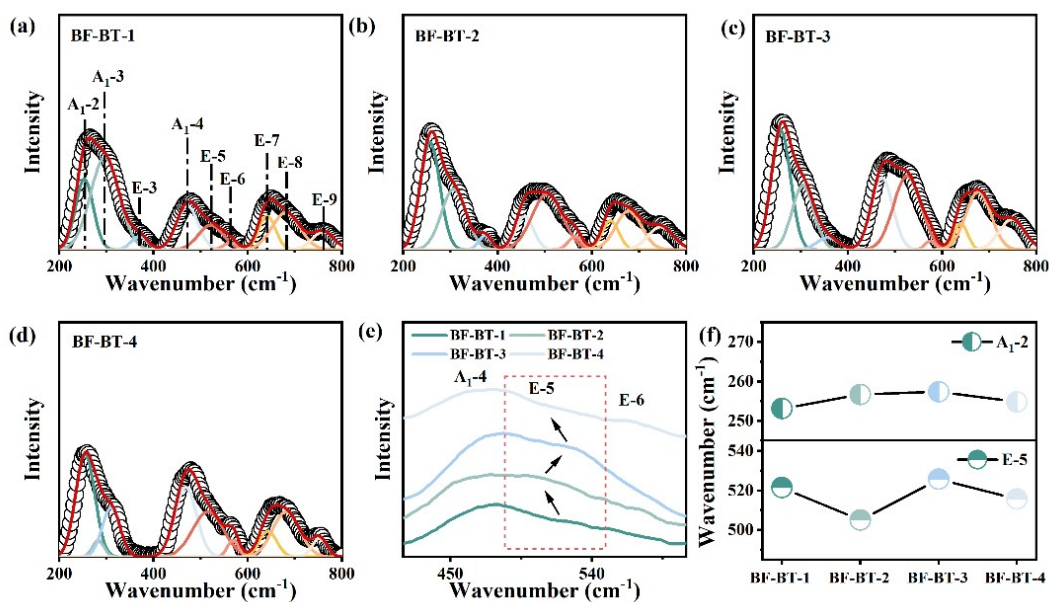
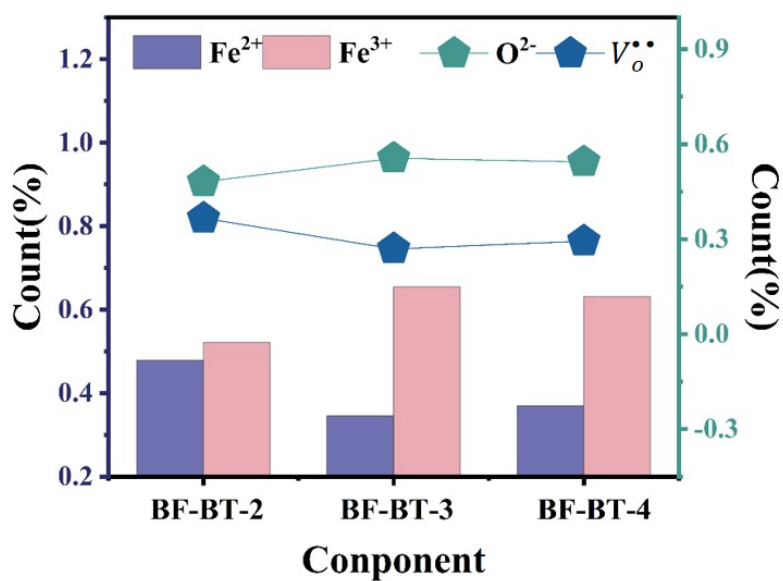


Fig. S2. (a-d) raman spectrum with Gaussian fitting curves; (e) the enlarged image of the E-5 peak; (f) content dependence of partial vibrational mode peaks.



Figs. S3 Fe²⁺/Fe³⁺ and O²⁻/V_o^{••} relative content of BF-BT-2, BF-BT-3, and BF-BT-4;

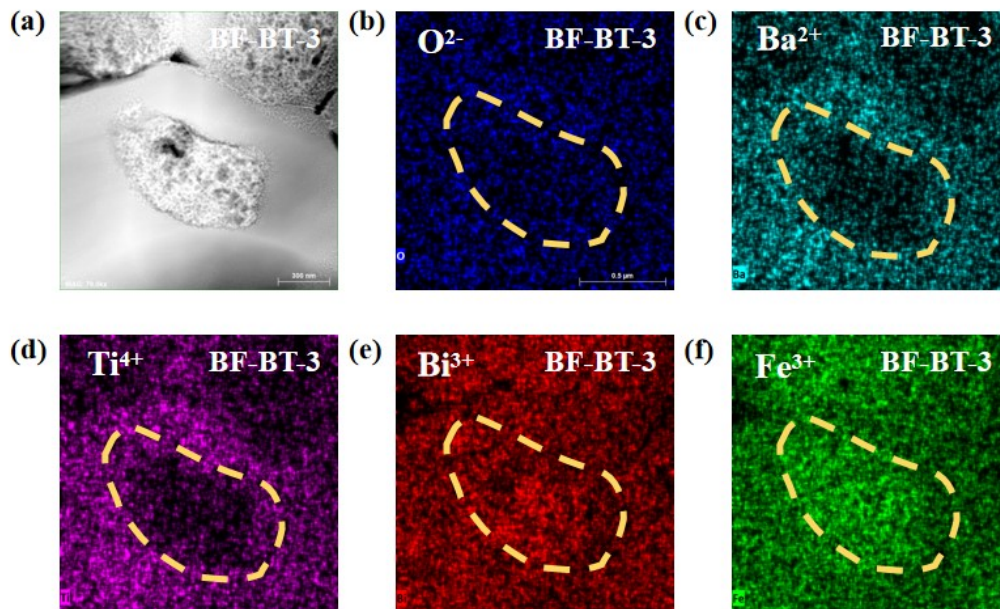


Fig. S4. (a-f) elemental distribution comparative mapping of Bi, Fe, Ba and Ti of BF-BT-3

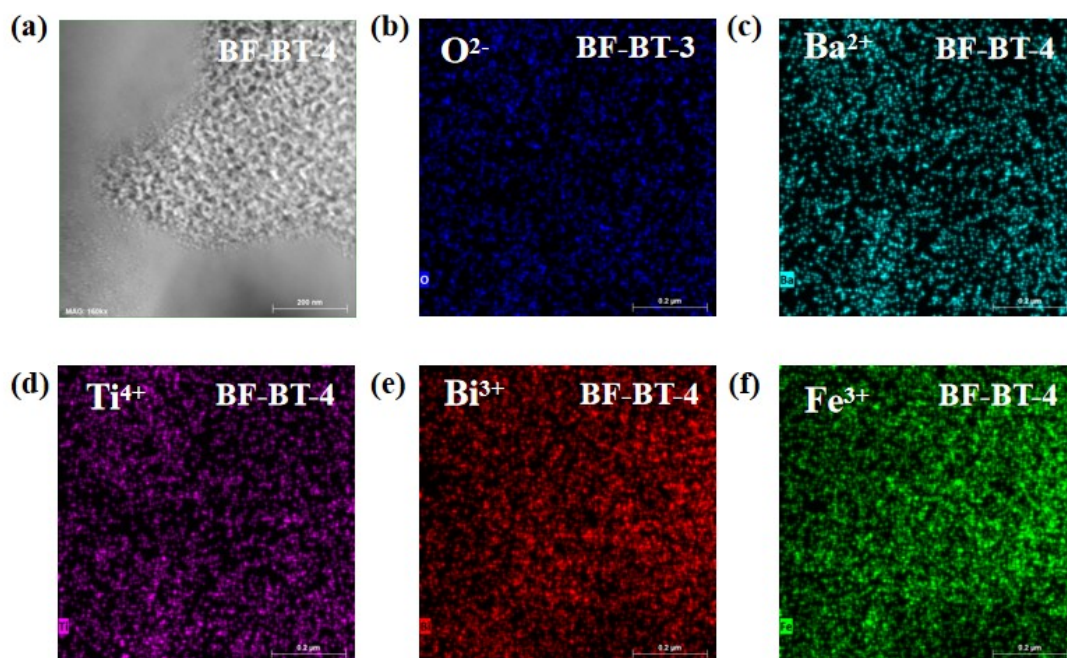


Fig. S5. (a-f) elemental distribution comparative mapping of Bi, Fe, Ba and Ti of BF-BT-4.

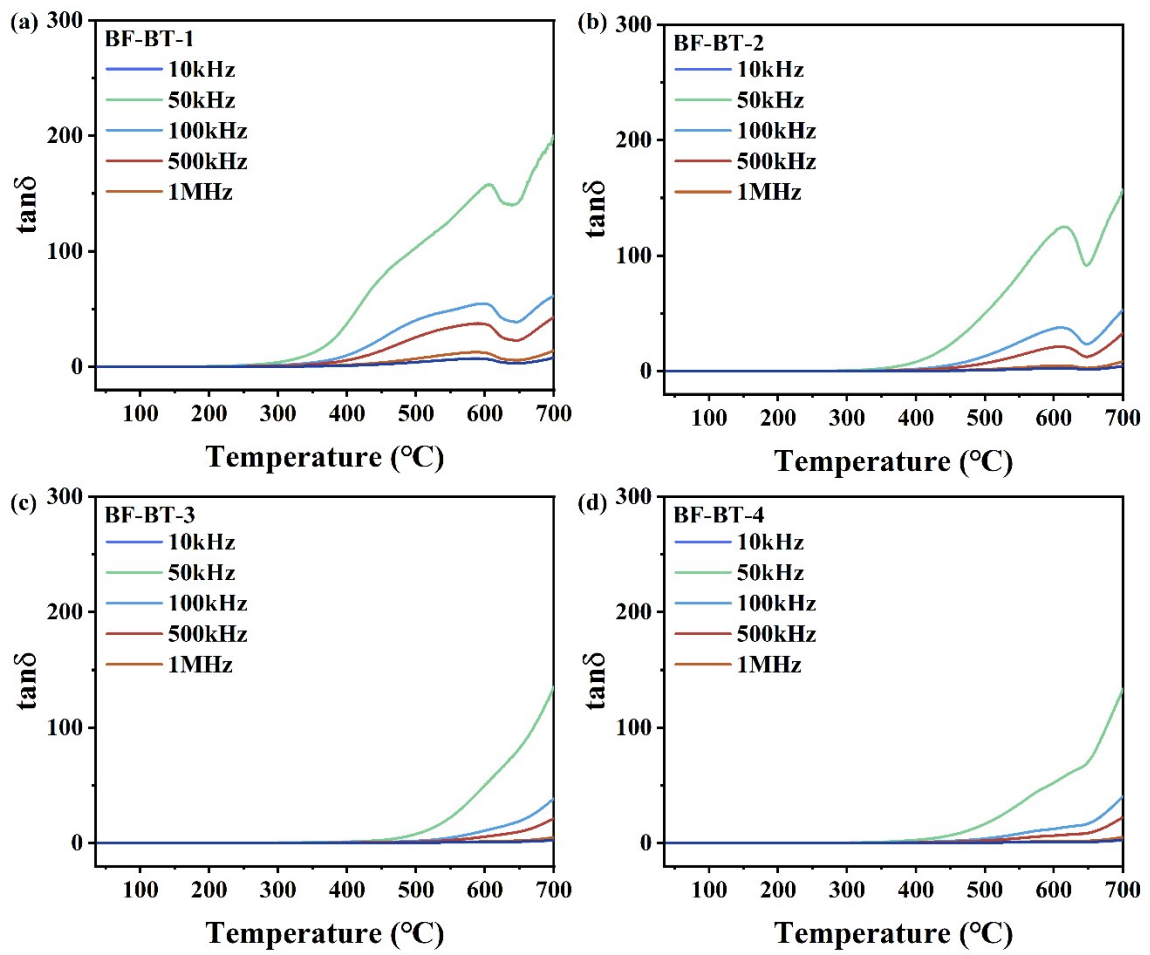


Fig. S6 The $\tan\delta$ -T curves of BF-BT-1, BF-BT-2, BF-BT-3 and BF-BT-4.

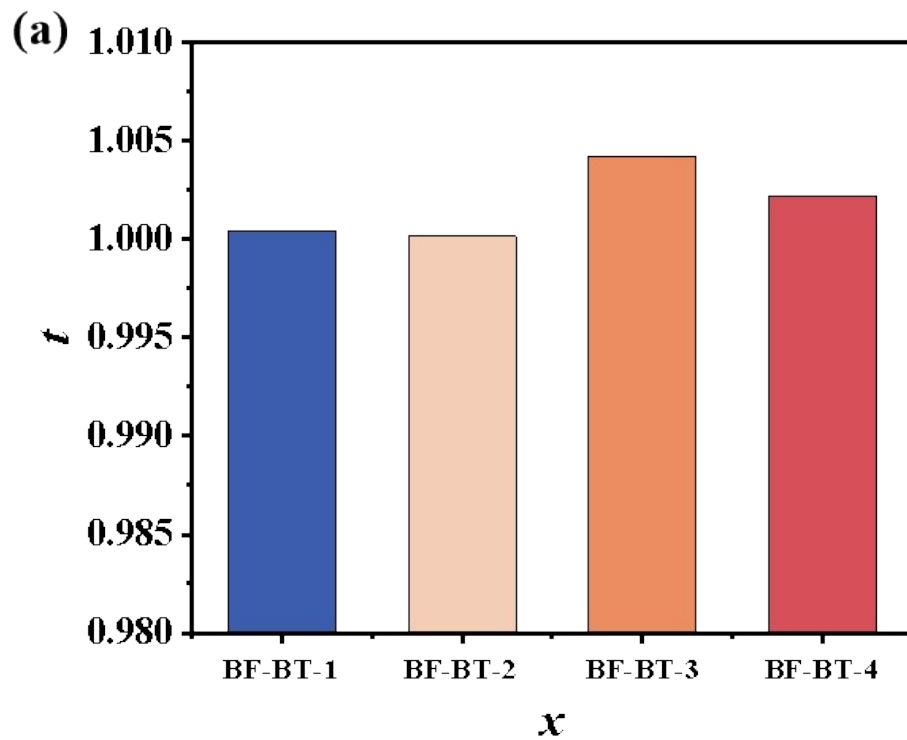
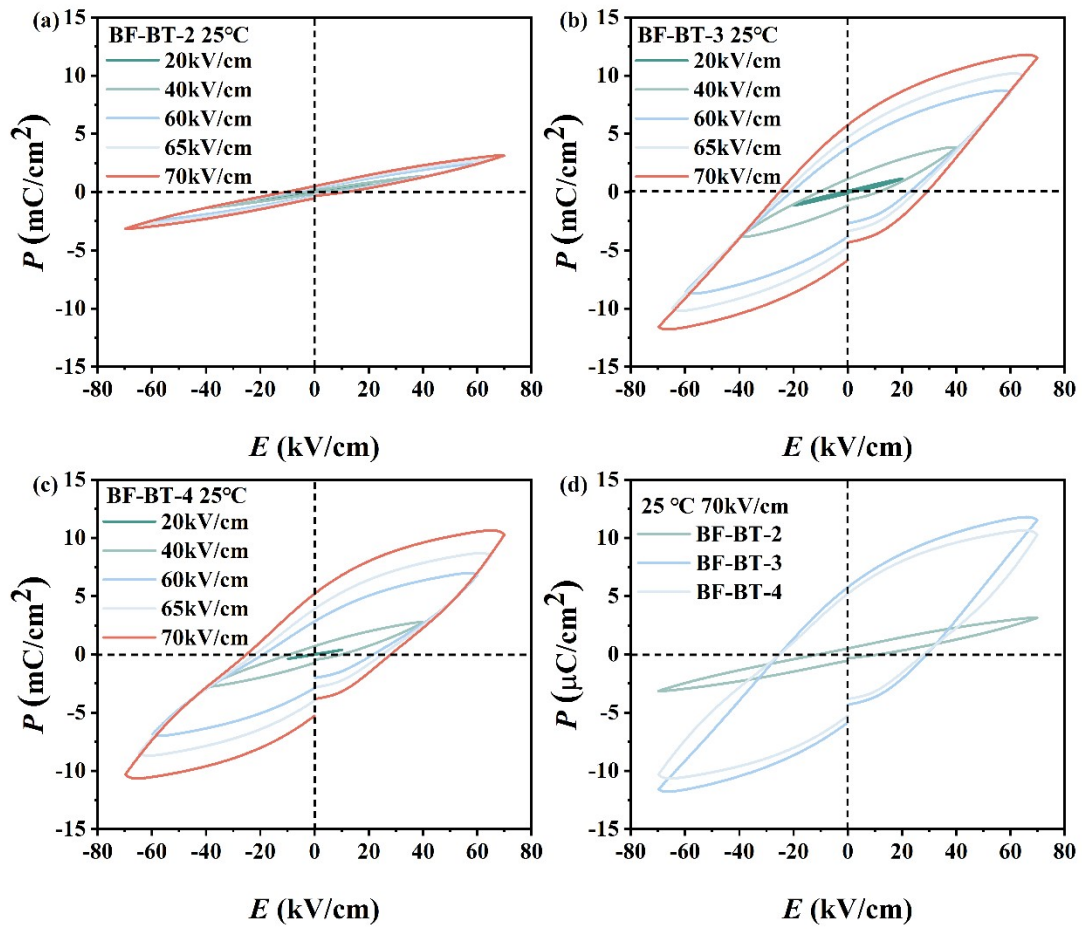


Fig. S7. (a) the tolerance factor t of BF-BT-1, BF-BT-2, BF-BT-3 and BF-BT-4.



Figs. S8 (a-c) The hysteresis loops of BF-BT-2, BF-BT-3, and BF-BT-4 at room temperature (d) The component-dependent room-temperature hysteresis loops under the 70 kV/cm electric field.