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Electronic Supplementary Information

Series of High-Temperature Molecular ferroelectric crystals: Chlorine doped Diisopropylammonium Bromide

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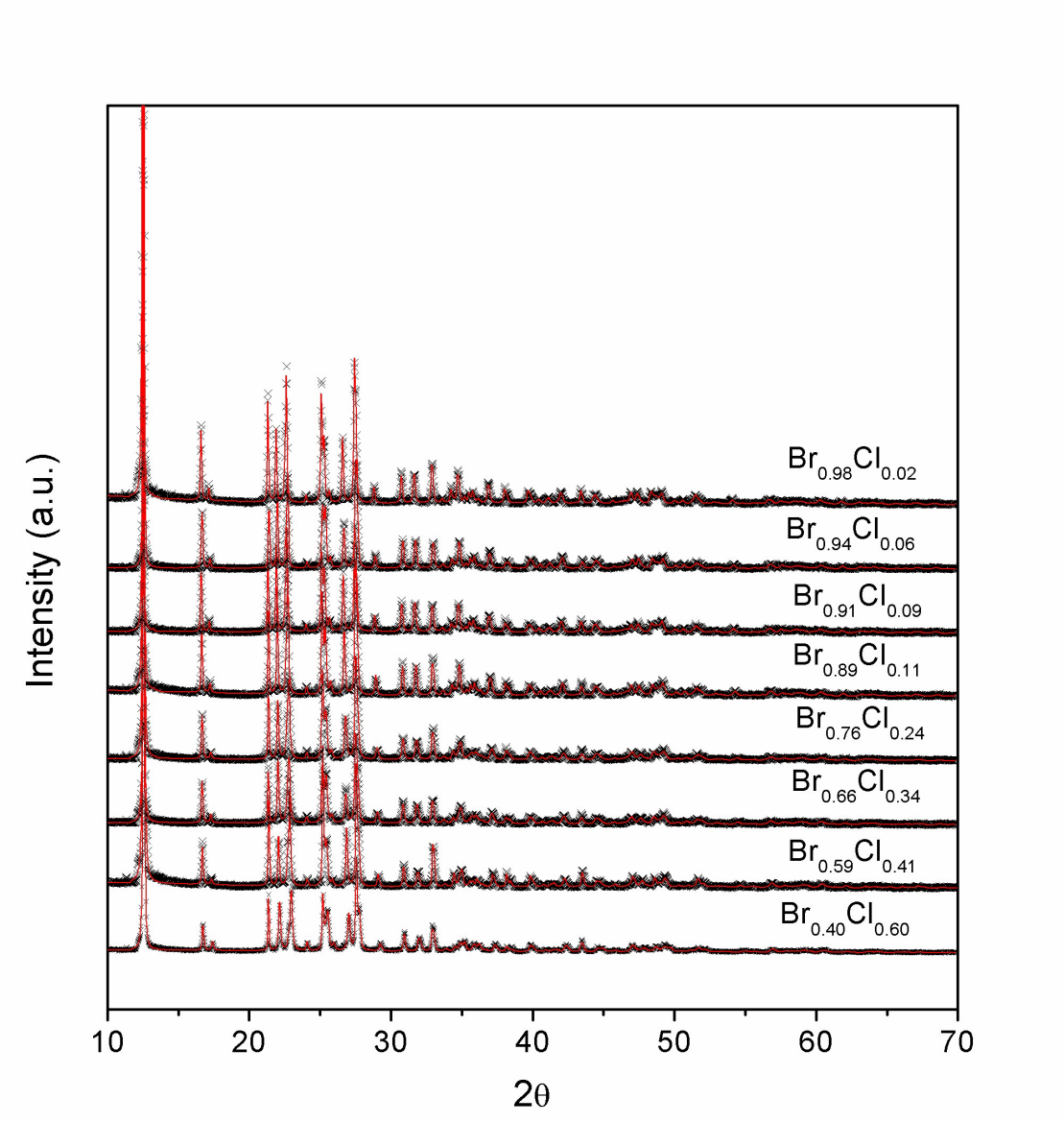

Fig. S1. Rietveld refinements of PXRD pattern of the obtained chlorine doped DIPAB

with $P2_1$ phase. The black "×" represents the measured XRD pattern and the red line is the refinement curve.

Table S1 The lattice parameters and r_{wp} of the chlorine doped DIPAB samples got by the Rietveld refinements of PXRD pattern

Measured chlorine content x	a	b	c	β	volume	r_{wp}
0	7.8614(6)	8.0978(5)	7.8943(6)	116.280(5)	450.61(6)	10.83%
0.02	7.8661(3)	8.1092(3)	7.9038(2)	116.272(2)	452.10(3)	10.04%
0.06	7.8665(3)	8.1096(2)	7.9067(2)	116.250(2)	452.39(2)	8.24%
0.09	7.8605(3)	8.1062(3)	7.9000(2)	116.192(2)	451.69(3)	9.55%
0.11	7.8541(3)	8.0991(3)	7.8984(2)	116.116(2)	451.13(2)	9.87%
0.24	7.8288(4)	8.0812(4)	7.8780(3)	115.953(3)	448.15(4)	9.92%
0.34	7.8275(4)	8.0798(3)	7.8796(3)	115.889(3)	448.32(3)	9.51%
0.41	7.8105(4)	8.0651(5)	7.8631(2)	115.868(3)	445.69(4)	10.99%
0.60	7.7472(4)	8.0100(4)	7.8165(3)	115.528(3)	437.70(4)	9.88%

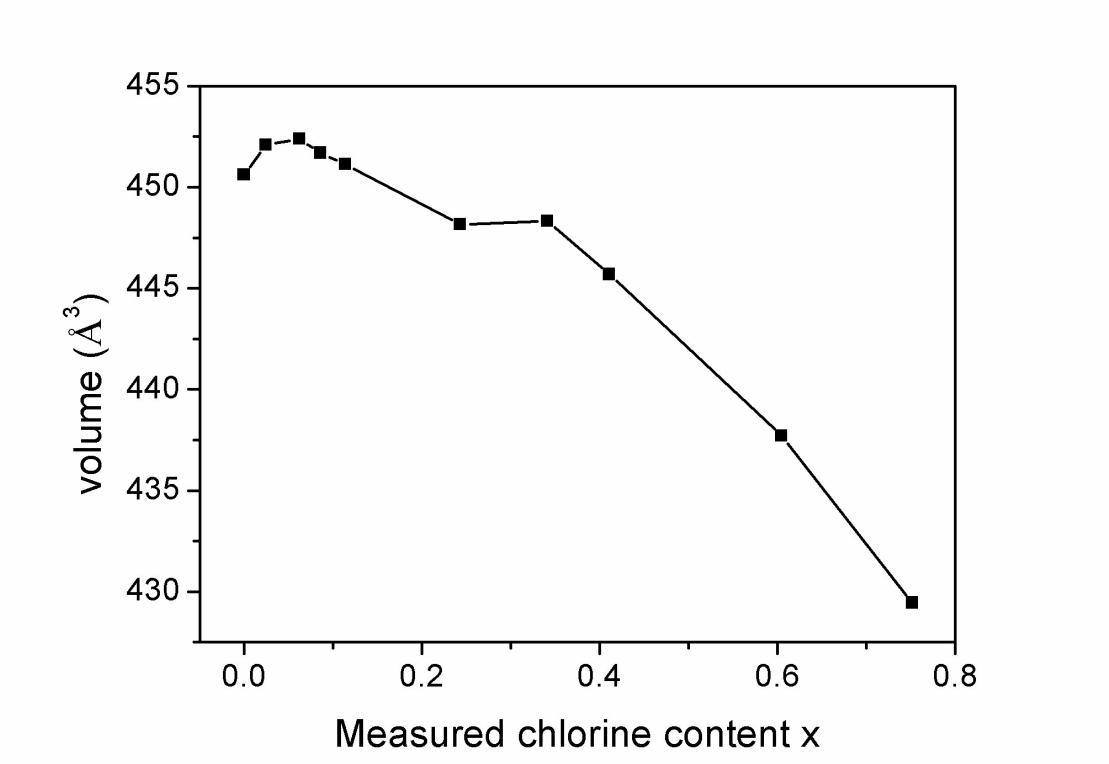

Fig. S2 The unit cell volume of the chlorine doped DIPAB versus the measured chlorine content.

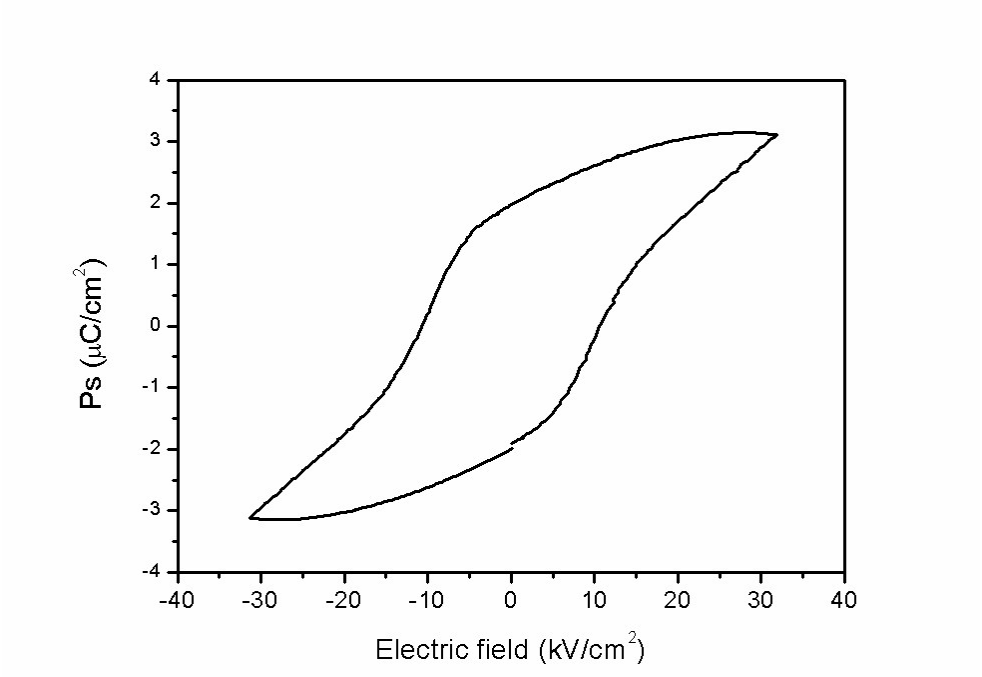

Fig. S3 The ferroelectric hysteresis loop of $C_6H_{16}NBr_{0.59}Cl_{0.41}$ at 423K.