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Supporting Information for Publication

Novel Organic-Inorganic Hybrid Ferroelectric; bis(imidazolium) pentachloroantimonate(III), $(C_3N_2H_5)_2SbCl_5$

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Table S1. Selected bond lengths (Å) and angles (deg) for ICA at 193(2) and 100(2) K.

193 K		**100 K**	
Sb-Cl(1)	2.4232(9)	Sb(1)-Cl(1)	2.4279(6)
Sb-Cl(2)	2.4429(8)	Sb(1)-Cl(2)	2.4392(5)
Sb-Cl(3)	2.5461(8)	Sb(1)-Cl(3)	2.5999(6)
Sb-Cl(4)	2.7281(9)	Sb(1)-Cl(4)	2.6447(6)
		Sb(1A)-Cl(1A)	2.4195(6)
		Sb(1A)-Cl(2A)	2.4507(5)
		Sb(1A)-Cl(3A)	2.4968(6)
		Sb(1A)-Cl(4A)	2.8142(6)
Cl(1)-Sb-Cl(2)	92.33(3)	Cl(1)-Sb(1)-Cl(2)	92.94(2)
Cl(1)-Sb-Cl(3)	88.94(3)	Cl(1)-Sb(1)-Cl(3)	87.90(2)
Cl(2)-Sb-Cl(3)	89.71(3)	Cl(2)-Sb(1)-Cl(3)	89.22(2)
Cl(1)-Sb-Cl(4)	88.86(3)	Cl(1)-Sb(1)-Cl(4)	89.08(2)
Cl(2)-Sb-Cl(4)	87.74(3)	Cl(2)-Sb(1)-Cl(4)	87.88(2)
Cl(3)-Sb-Cl(4)	176.55(2)	Cl(3)-Sb(1)-Cl(4)	175.707(17)
		Cl(1A)-Sb(1A)-l(2A)	92.24(2)
		Cl(1A)-Sb(1A)-l(3A)	89.964(19)
		Cl(2A)-Sb(1A)-l(3A)	90.01(2)
		Cl(1A)-Sb(1A)-l(4A)	88.629(19)
		Cl(2A)-Sb(1A)-l(4A)	87.26(2)
		Cl(3A)-Sb(1A)-l(4A)	176.877(16)

Table S2. Hydrogen bonds in ICA (Å) and (deg) at 1933(2) and 100(2) K.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
193 K				
N(1)-(1)...Cl(2)	0.88	2.72	3.484(6)	145.9
N(1A)-(1A)...Cl(4)^{ii}	0.88	2.93	3.412(13)	115.9
N(11)-H(11)...Cl(5)	0.88	2.56	3.351(3)	150.4
N(11)-(11)...Cl(3)^{iii}	0.88	2.87	3.395(4)	120.2
N(21)-(21)...Cl(4)^{iv}	0.88	2.36	3.237(3)	172.1
N(23)-H(23)...Cl(3)	0.88	2.64	3.304(3)	132.6
N(23)-H(23)...Cl(6)	0.88	2.67	3.365(3)	136.2
100 K				
N(1)-H(1)...Cl(6)	0.88	2.52	3.267(2)	142.9
N(1)-H(1)...Cl(2)	0.88	2.95	3.489(2)	121.2
N(3)-(3)...Cl(4A)^{i}	0.88	2.26	3.118(2)	165.5
N(11)-H(11)...Cl(5)	0.88	2.45	3.276(2)	157.5
N(11)-(11)...Cl(3A)^{ii}	0.88	2.95	3.415(2)	114.5
N(13)-H(13)...Cl(5)^{iii}	0.88	2.62	3.357(2)	142.1
N(13)-H(13)...Cl(3)^{iii}	3 0.88	2.72	3.295(2)	124.0
N(21)-H(21)...Cl(4)^{iv}	0.88	2.36	3.232(2)	171.7
N(23)-H(23)...Cl(6)	0.88	2.62	3.332(2)	138.1
N(23)-H(23)...Cl(3)	0.88	2.62	3.276(2)	132.3
N(31)-(31)...Cl(4A)^{v}	0.88	2.36	171.4	3.233(2)
N(33)-H(33)...Cl(6)	0.88	2.64	3.329(2)	135.4
N(33)-H(33)...Cl(3A)	0.88	2.65	3.315(2)	133.5

Symmetry transformations used to generate equivalent atoms: 193 K: *(ii)* -x+1/2, y-1/2, z ;
(iii) -x+1,-y+1,-z *(iv)* x+1, y, z; 100 K: *(i)* -x+3/2,y-1/2,z+1/2 *(ii)* x-1/2,-y+3/2,z *(iii)* x+1/2,-y+3/2,z *(iv)* x,y,z-1 *(v)* x,y,z+1

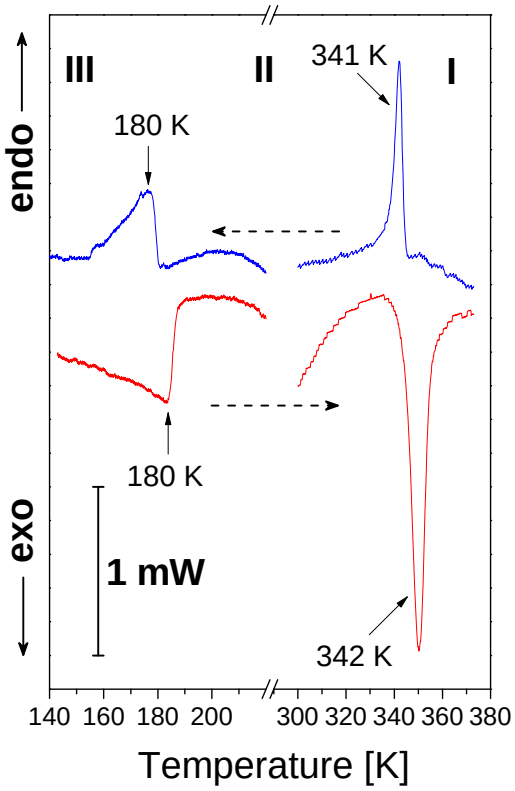

Figure S1 DSC curves for the ICA crystal upon cooling and heating runs (10 K min^{-1}, m = 19 mg).

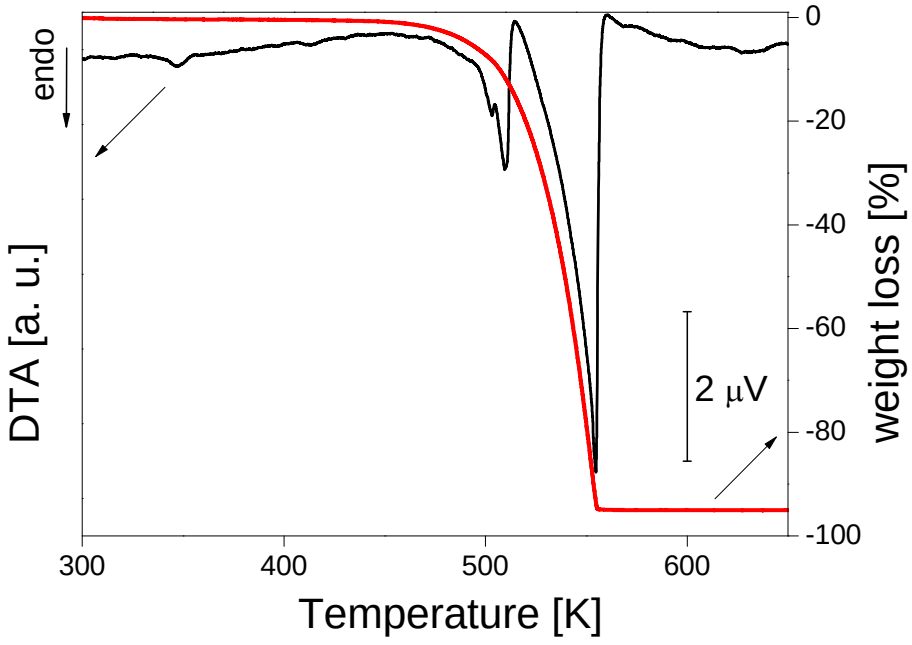

Figure S2 Simultaneous thermogravimetric analysis and thermal analysis scan (with temperature rate of 2 K min^{-1}, sample mass 15.7 mg) for ICA