New sarcosine-metal halide complexes related to the ferroelectric TSCC

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Supplementary Material

Crystallographic data

Table S1 Crystallographic data and refinement details collected at 173 K

Parameter	TSCB	TSSC	TSSB	TSMnI	TSMgB	BSCl	BSMgC	BSMnC	TSCl
Formula	$(C_3NO_2H_7)_3CaBr_2$	$(C_3NO_2H_7)_3SrCl_2$	$(C_3NO_2H_7)_3SrBr_2$	$(C_3NO_2H_7)_3MnI_2.2H_2O$	$(C_3NO_2H_7)_3MgBr_2.2H_2O$	$(C_3NO_2H_7)_2CaI_2.2H_2O$	$(C_3NO_2H_7)_2MgCl_2.2H_2O$	$(C_3NO_2H_7)_2MnCl_2.2H_2O$	$(C_3NO_2H_7)_4CaI_2.2H_2O$
Formula Weight	467.19	425.81	514.73	612.06	487.45	508.10	309.43	340.06	686.29
Density (g cm^{-3})	1.832	1.747	2.022	2.093	1.793	2.066	1.520	1.630	1.792
Crystal System	Orthorhombic	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic	Triclinic	Triclinic	Triclinic	Monoclinic
Space Group	Pnma	$P2_1/a$	Pcab	Pnma	Pnma	P-1	P-1	P-1	$P2_1/n$
a/Å	9.2414(6)	8.7535(6)	8.7723(6)	9.8288(7)	9.5844(6)	4.9952(4)	4.7711(4)	4.8078(4)	11.2880(8)
b/Å	17.6966(13)	10.3752(7)	10.5359(7)	19.2160(15)	18.9445(13)	5.9493(5)	5.3186(4)	5.3548(4)	10.0620(7)
c/Å	10.3565(7)	17.8337(13)	36.5820(3)	10.2845(8)	9.9448(6)	13.8126(12)	13.5193(12)	13.6620(12)	23.0573(16)
α/°	90	90	90	90	90	95.593(13)	84.365(12)	83.825(12)	90
β/°	90	91.867(6)	90	90	90	90.980(12)	82.080(12)	82.288(12)	103.722(4)
γ/°	90	90	90	90	90	90.965(11)	87.969(12)	87.503(12)	90
V/$Å^3$	1693.7(2)	1618.8(2)	3381.1(3)	1942.4(3)	1805.7(2)	408.40(6)	338.06(5)	346.37(5)	2544.1(3)
Z	4	4	8	4	4	1	1	1	4
Measured Ref	15967	16382	21461	18998	17644	4214	3423	3548	25445
Independent Ref	1969 [R(int) = 0.0500]	3726 [R(int) = 0.0856]	3873 [R(int) = 0.0518]	2301 [R(int) = 0.0992]	2139 [R(int) = 0.0624]	1859 [R(int) = 0.0589]	1536 [R(int) = 0.0467]	1574 [R(int) = 0.0497]	5835 [R(int) = 0.0639]
Refined Parameter	149	274	274	147	166	96	96	115	393
GOOF	0.800	0.823	1.015	0.978	0.794	1.107	1.639	0.815	0.878
Final R Indices (I > 2σ(I))	R1 = 0.0274	R1 = 0.0390	R1 = 0.0307	R1 = 0.0406	R1 = 0.0288	R1 = 0.0659	R1 = 0.0625	R1 = 0.0429	R1 = 0.0392

Table S2 Crystallographic data and refinement details of strontium doped TSCC and TSCB

Parameter	TSCC 50% Sr	TSCB 50% Sr
Formula	$(C_3NO_2H_7)_3Ca_{0.5}Sr_{0.5}Cl_2$	$(C_3NO_2H_7)_3Ca_{0.5}Sr_{0.5}Br_2$
Formula Weight	398.71	486.60
Density (g cm^{-3})	1.620	1.895
Crystal System	Orthorhombic	Orthorhombic
Space Group	Pnma	Pnma
a/Å	8.9965(7)	9.1728(7)
b/Å	17.6045(3)	17.8422(14)
c/Å	10.3191(15)	10.4200(8)
α/°	90	90
β/°	90	90
γ/°	90	90
V/$Å^3$	1634.3(3)	1705.4(2)

Z	4	4
Measured Ref	15958	16650
Independent Ref	1926 [R(int) = 0.0732]	2020 [R(int) = 0.0841]
Refined Parameter	150	150
GOOF	1.079	0.895
Final R Indices (I > 2σ(I))	R1 = 0.0522	R1 = 0.0384

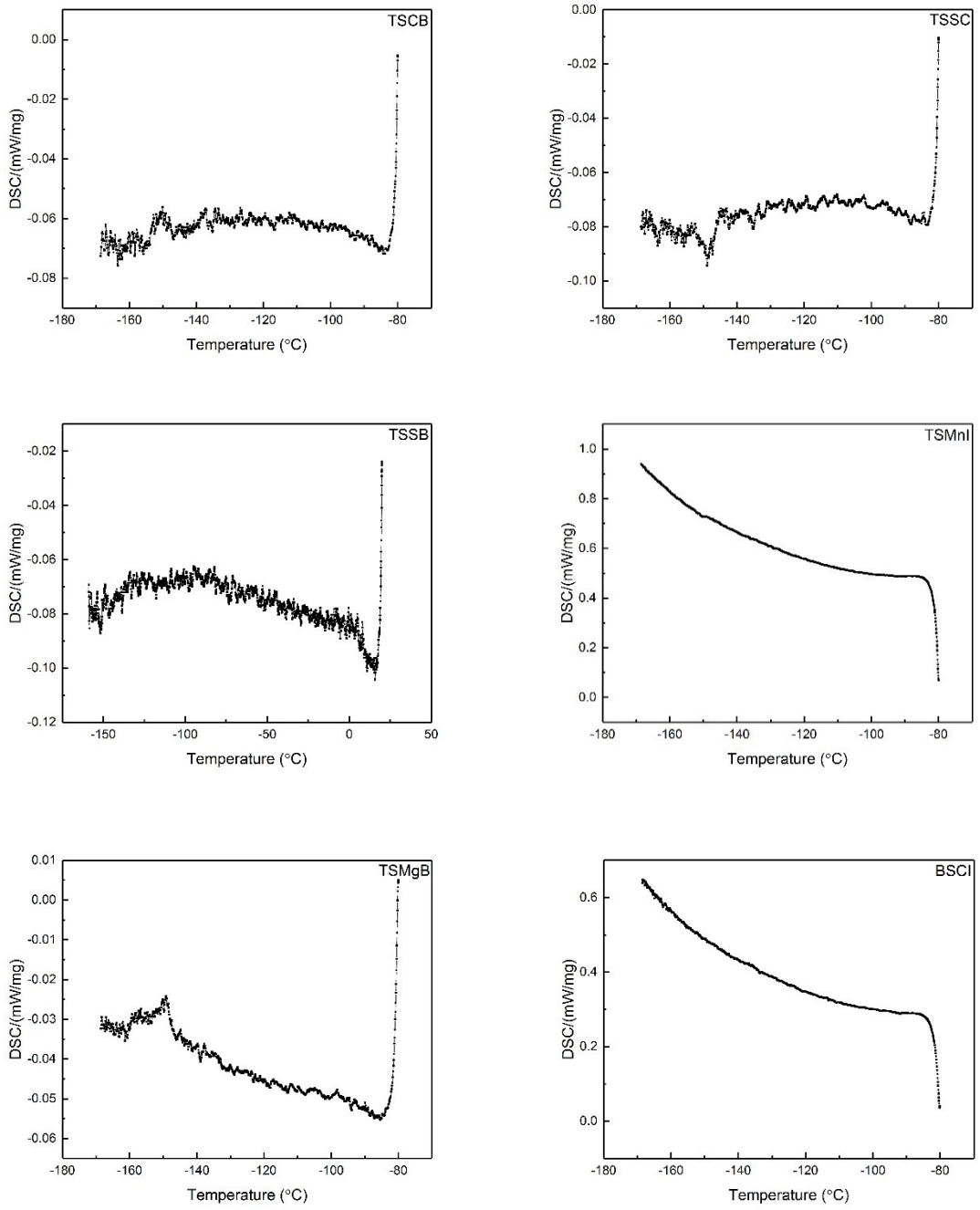
Table S3 Selected bond distances (Å) and bond valence sums derived from single crystal X-ray diffraction data collected at 173 K

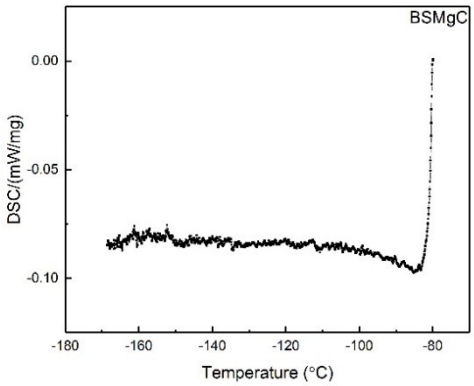
Bond	TSCB	TSSC	TSSB	TSMnI	TSMgB	BSCl	BSMgC	BSMnC	TSCl	
M - O	2.2935(15)	2.431(3)	2.438(3)	2.155(6)	2.019(3)	2.335(6)	2.066(4)	2.150(2)	2.292(3)	2.304(3)
	2.2936(15)	2.500(3)	2.518(36)	2.192(6)	2.082(2)	2.335(6)	2.066(4)	2.150(2)	2.292(3)	2.304(3)
	2.305(2)	2.537(3)	2.521(3)	2.200(4)	2.082(2)	2.338(7)	2.073(4)	2.173(3)	2.323(3)	2.328(3)
	2.3671(19)	2.568(3)	2.572(2)	2.200(4)	2.096(2)	2.338(7)	2.073(4)	2.173(3)	2.323(3)	2.328(3)
	2.3816(14)	2.583(3)	2.595(3)	2.208(4)	2.096(2)	2.394(10)	2.102(4)	2.202(2)	2.392(3)	2.399(3)
	2.3816(14)	2.721(3)	2.660(3)	2.208(4)	2.102(3)	2.394(10)	2.102(4)	2.202(2)	2.392(3)	2.399(3)
		2.796(3)	2.888(3)							
N-H-X	3.2864(12)	3.163(4)	3.288(3)	3.503(4)	3.3203(17)	3.483(8)	3.124(4)	3.146(3)	3.561(4)	
	3.3188(17)	3.210(4)	3.355(3)	3.549(5)	3.422(3)	3.462(9)	3.079(5)	3.098(3)	3.612(4)	
	3.3287(18)	3.173(4)	3.293(3)	3.692(5)	3.483(3)				3.577(5)	
		3.234(4)	3.374(3)						3.487(5)	
		3.226(4)	3.320(3)							
		3.251(4)	3.311(3)							
BVS	2.22	2.04	2.01	2.02	2.12	2.10	2.11	2.12	2.23	2.18

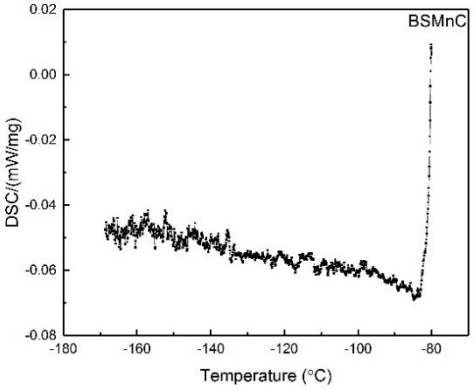
Table S4 Selected bond distances (Å) of strontium doped TSCC and TSCB

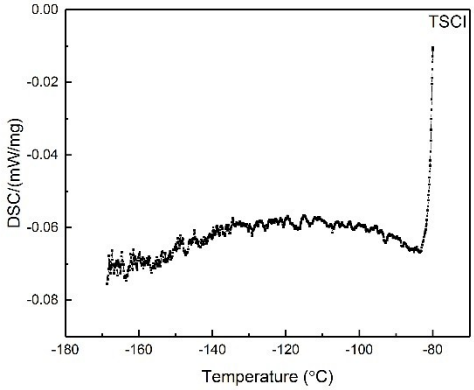
Bond	TSCC 50% Sr	TSCB 50% Sr
M - O	2.341(3)	2.324(4)
	2.341(3)	2.324(4)
	2.346(4)	2.344(5)
	2.430(4)	2.428(5)
	2.448(3)	2.444(4)
	2.448(3)	2.444(4)
N-H-X	3.206(2)	3.306(3)
	3.233(3)	3.334(5)
	3.224(3)	3.345(5)

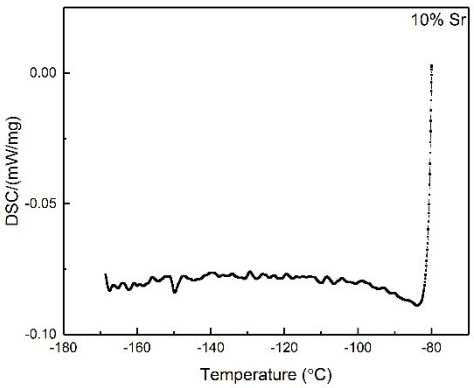
Figure S1 Differential Scanning Calorimetry data of TSCB ($(C_3NO_2H_7)_3CaBr_2$), TSSC ($(C_3NO_2H_7)_3SrCl_2$), TSSB ($(C_3NO_2H_7)_3SrBr_2$), TSMnI ($(C_3NO_2H_7)_3MnI_2.2H_2O$), TSMgB ($(C_3NO_2H_7)_3MgBr_2.2H_2O$), BSCl ($(C_3NO_2H_7)_2CaI_2.2H_2O$), BSMgC ($(C_3NO_2H_7)_2MgCl_2.2H_2O$), BSMnC ($(C_3NO_2H_7)_2MnCl_2.2H_2O$), TSCl ($(C_3NO_2H_7)_4CaI_2.2H_2O$), TSCC 10% Sr ($(C_3NO_2H_7)_3Ca_{0.9}Sr_{0.1}Cl_2$), TSCC 20% Sr ($(C_3NO_2H_7)_3Ca_{0.8}Sr_{0.2}Cl_2$) and TSCC 30% Sr ($(C_3NO_2H_7)_3Ca_{0.7}Sr_{0.3}Cl_2$).

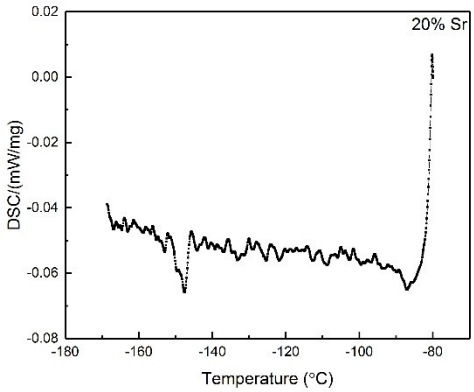



BSMgC
DSC/(mW/mg)
0.00
-0.05
-0.10
-180
-160
-140
-120
-100
-80
Temperature (°C)


BSMnC
DSC/(mW/mg)
0.02
0.00
-0.02
-0.04
-0.06
-0.08
-180
-160
-140
-120
-100
-80
Temperature (°C)


TSCI
DSC/(mW/mg)
0.00
-0.02
-0.04
-0.06
-0.08
-180
-160
-140
-120
-100
-80
Temperature (°C)


10% Sr
DSC/(mW/mg)
0.00
-0.05
-0.10
-180
-160
-140
-120
-100
-80
Temperature (°C)


20% Sr
DSC/(mW/mg)
0.02
0.00
-0.02
-0.04
-0.06
-0.08
-180
-160
-140
-120
-100
-80
Temperature (°C)

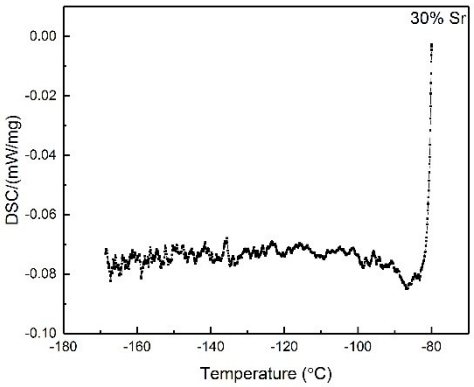
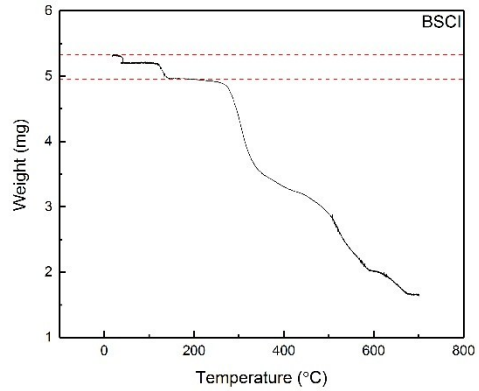
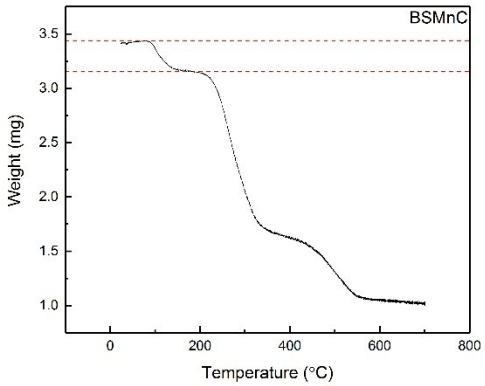

30% Sr
DSC/(mW/mg)
0.00
-0.02
-0.04
-0.06
-0.08
-0.10
-180
-160
-140
-120
-100
-80
Temperature (°C)

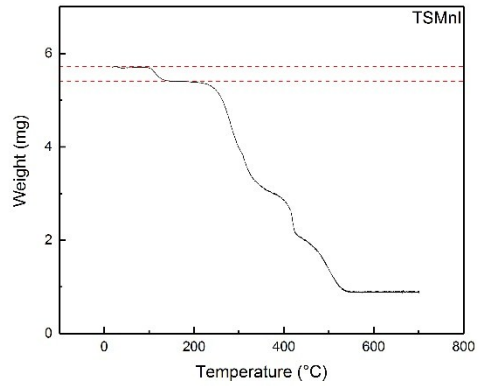
Figure S2 Thermal Gravimetric Analysis data of BSCl ($(C_3NO_2H_7)_2CaI_2.2H_2O$), BSMnC ($(C_3NO_2H_7)_2MnCl_2.2H_2O$) and TSMnI ($(C_3NO_2H_7)_3MnI_2.2H_2O$) showing observed and theoretical weight loss corresponding to dehydration



% weight loss = 6.99 %
Theoretical weight loss = 7.09 %



% weight loss = 8.15 %
Theoretical weight loss = 10.59 %



% weight loss = 5.59 %
Theoretical weight loss = 5.89 %