Electronic Supplementary Material (ESI) for RSC Advances.

A multi-functional iodoplumbate-based hybrid crystal: 1-propyl-4-aminopyridinium triiodoplumbate

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Preparation of 1

A mixture of PbI_2 (0.926 g, 2 mmol) and KI (3.320 g, 20 mmol) with molar ratio of 1:10 in DMF (50 mL) was heated under reflux with stirring for 25 min. After the clear yellow solution was formed and a DMF solution [C_3-Apy]Br (2 mmol) was slowly added to the mixture, which was stirred for 8 h and filtered to remove insoluble compounds. The filtrate was evaporated at ambient temperature for 14 days to produce light yellowish needle-shaped crystals in ca. 75% yield. The crystal was washed with DMF.

Table S1 Crystallographic data and refinement parameter of **1** at room temperature

Temperature (K)	293(2)	120(2)
Wavelength (Å)	0.71073	0.71073
Empirical formula	$C_{16}H_{26}I_6N_4Pb_2$	$C_{16}H_{26}I_6N_4Pb_2$
Formula weight	1450.2	1450.2
CCDC no.	1509582	1510132
Crystal system	Orthorhombic	Orthorhombic
Space group	Pnma	Pnma
a (Å)	7.8748(5)	7.8013(11)
b (Å)	10.4050(8)	10.2985(15)
c (Å)	19.3554(17)	19.117(3)
α (°)	90	90
β (°)	90	90
γ (°)	90	90
V (Å^3)/Z	1585.9(2))/2	1535.9(4)/2
ρ (g·cm^{-1})	3.307	3.136
F(000)	1264.0	1264.0
Abs. coeff. (mm^{-1})	16.452	16.988
θ Ranges (data collection; °)	2.29 - 25.67	2.15 - 27.57
Index ranges	$-9 \le h \le 9$	$-10 \le h \le 10$
	$-10 \le k \le 12$	$-13 \le k \le 13$
	$-23 \le l \le 19$	$-24 \le l \le 24$
R_{int}	0.1229	0.0435
Independent reflections/restraints/param	1596/0/102	1870/0/83

eters		
Goodness of fit on F^2	1.082	1.287
R_1, wR_2[a] [$I>2\sigma$(I)]	0.0832, 0.2296	0.0231, 0.0565
R_1, wR_2[a] [all data]	0.0949, 0.2460	0.0283, 0.0584
Residual (e·nm^{-3})	4.721/-2.636	0.995/-1.660

[a] $R_1 = \sum||F_o| - |F_c||/|F_o|$, $wR_2 = [\sum w(\sum F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S2 CIE coordinates of **1** at selected temperature

Temperature (K)	CIE coordinates
300	(0.462, 0.473)
275	(0.472, 0.478)
250	(0.483, 0.476)
225	(0.493, 0.474)
200	(0.504, 0.469)
175	(0.516, 0.461)
150	(0.521, 0.456)
125	(0.536, 0.445)
100	(0.550, 0.435)
85	(0.559, 0.427)
70	(0.569, 0.420)
55	(0.582, 0.409)
40	(0.591, 0.402)
25	(0.600, 0.394)
10	(0.606 ,0.389)

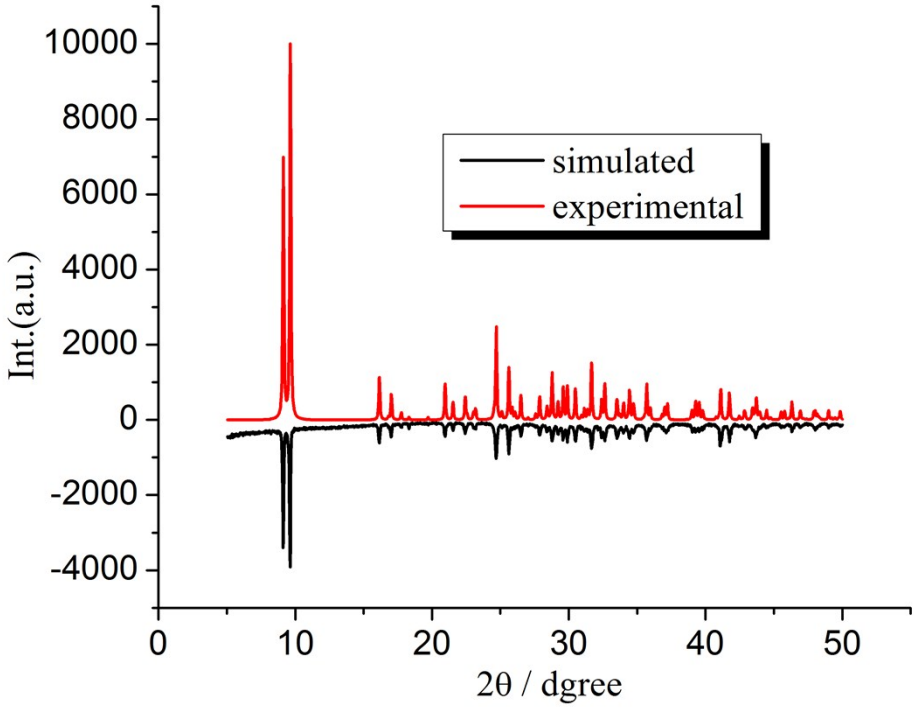

Figure S1 PXRD curve of **1** at room temperature

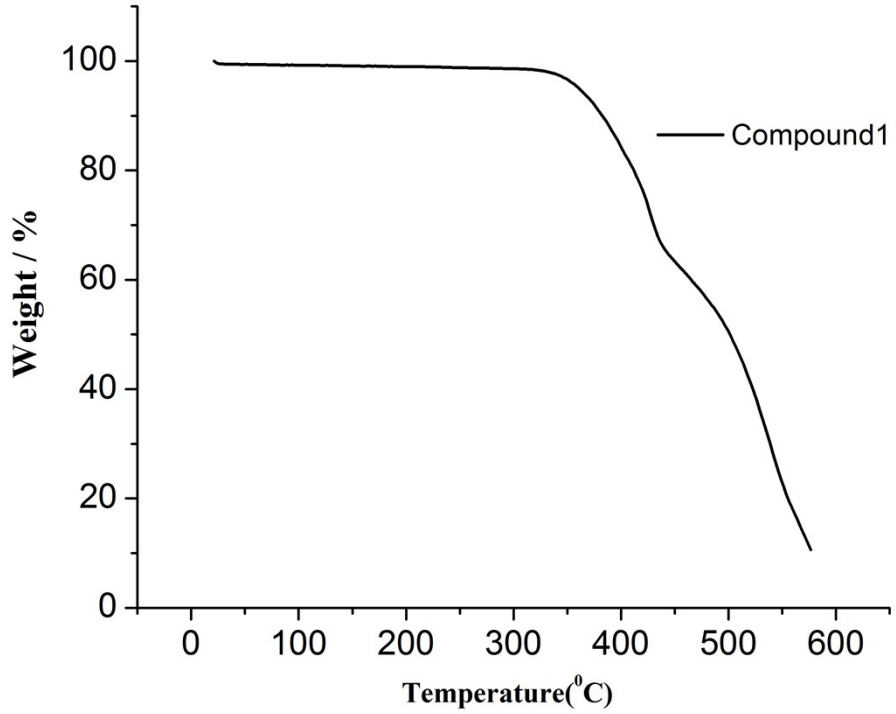

Figure S2 TG curve of **1**

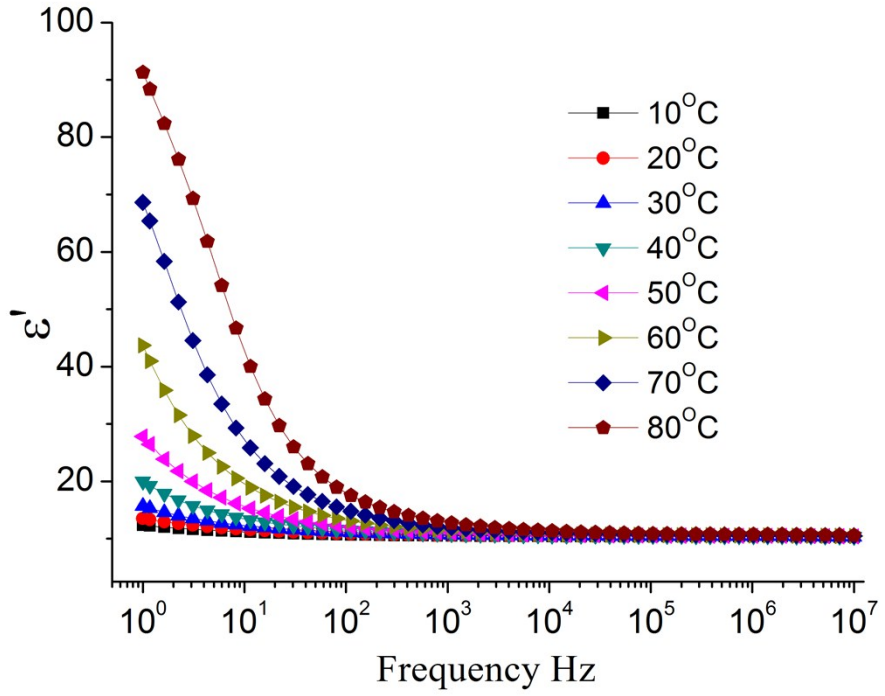

Figure S3 Frequency dependencies of the $\varepsilon'$of **1** in the 10-80 °C temperature range

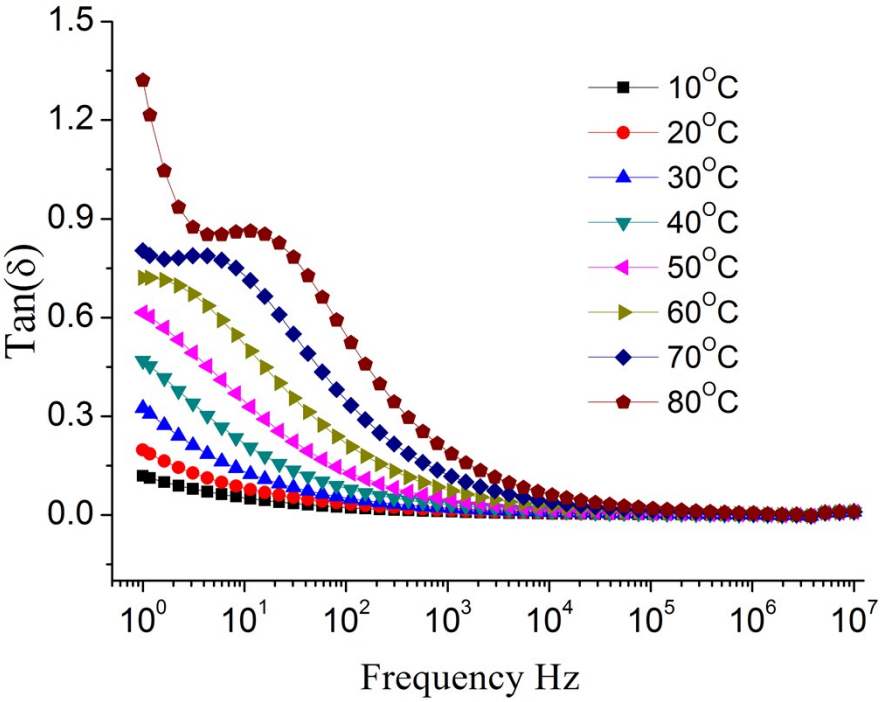

Figure S4 Frequency dependencies of *tan (δ)* of **1** in the 10-80 °C temperature range

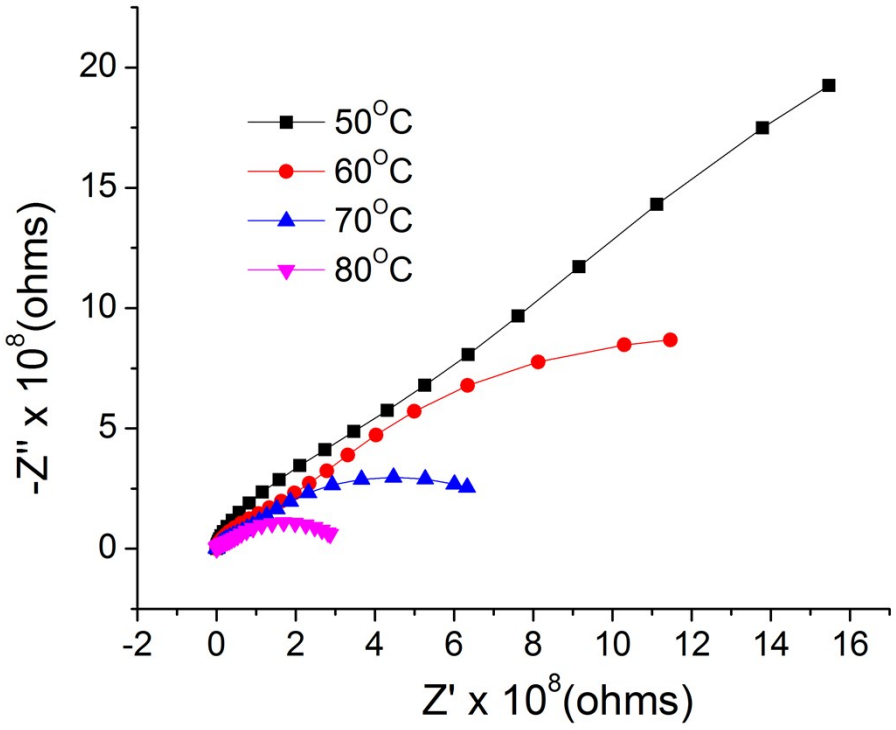

Figure S5 Complex impedance of **1** between 50 and 80 °C.

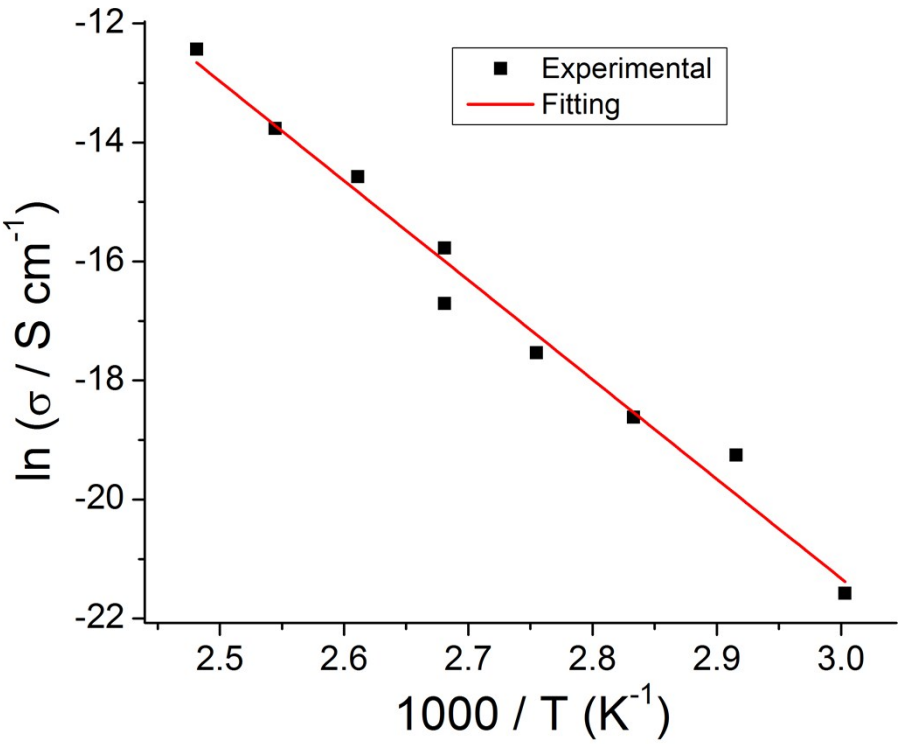

Figure S6 Arrhenius plots of **1** between 60 and 130 °C.

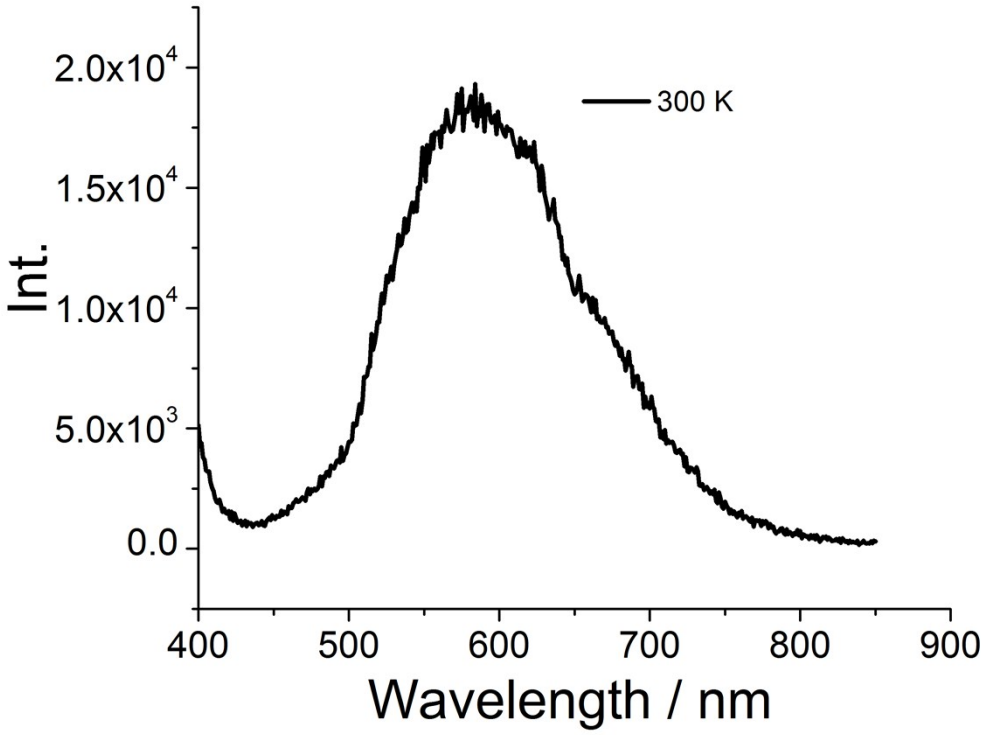

Figure S7 Emission spectra of **1** at room temperature