

An inorganic-organic hybrid crystal with two steps dielectric response and thermochromic luminescence

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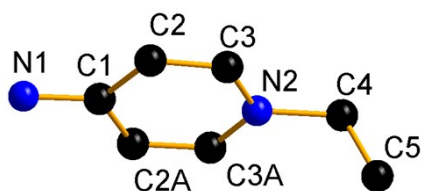
Table S1 Crystallographic data and refinement parameter of **1** at selected temperature

Temperature (K)	150	200	250	300	350
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Empirical formula	C ₇ H ₁₁ I ₃ N ₂ Pb	C ₇ H ₁₁ I ₃ N ₂ Pb	C ₇ H ₁₁ I ₃ N ₂ Pb	C ₇ H ₁₁ I ₃ N ₂ Pb	C ₇ H ₁₁ I ₃ N ₂ Pb
Formula weight	711.10	711.10	711.10	711.10	711.10
CCDC no.	1523553	1523554	1523555	1523556	1523557
Crystal system	orthorhombic	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>	<i>Pnma</i>
<i>a</i> (Å)	7.8023(9)	7.8158(8)	7.8294(7)	7.8382(6)	7.8530(15)
<i>b</i> (Å)	10.3378(12)	10.3604(10)	10.3796(9)	10.3922(7)	10.418(2)
<i>c</i> (Å)	18.120(2)	18.1750(18)	18.2256(16)	18.2707(13)	18.343(4)
<i>V</i> (Å ³)/ <i>Z</i>	1461.6(3) /4	1471.7(3) /4	1481.1(2) /4	1488.3(1)/4	1500.6(5)/4
ρ (g·cm ⁻³)	3.236	3.209	3.189	3.174	3.14
<i>F</i> (000)	1232	1232	1232	1232	1232
Abs. coeff. (mm ⁻¹)	17.849	17.726	17.61	17.57	17.38
θ Ranges (data collection; °)	0.993 - 27.67	0.996 - 27.65	0.991- 27.65	0.998- 25.00	0.999- 25.00
Index ranges	-10 ≤ <i>h</i> ≤ 10	-10 ≤ <i>h</i> ≤ 10	-10 ≤ <i>h</i> ≤ 10	-9 ≤ <i>h</i> ≤ 9	-9 ≤ <i>h</i> ≤ 9
	-13 ≤ <i>k</i> ≤ 13	-13 ≤ <i>k</i> ≤ 13	-13 ≤ <i>k</i> ≤ 13	-12 ≤ <i>k</i> ≤ 12	-12 ≤ <i>k</i> ≤ 12
	-23 ≤ <i>l</i> ≤ 23	-23 ≤ <i>l</i> ≤ 23	-23 ≤ <i>l</i> ≤ 23	-21 ≤ <i>l</i> ≤ 21	-21 ≤ <i>l</i> ≤ 21
Independent reflections/restraints/parameters	1790/0/71	1804/0/71	1804/0/71	1393/0/71	1403/0/71
Goodness of fit on <i>F</i> ²	1.103	1.077	1.127	1.041	1.448
<i>R</i> ₁ , <i>wR</i> ₂ ^a [<i>I</i> > 2σ(<i>I</i>)]	0.033, 0.087	0.0333, 0.0869	0.0347, 0.0906	0.0666, 0.1886	0.1457, 0.3697
<i>R</i> ₁ , <i>wR</i> ₂ ^a [all data]	0.037, 0.090	0.0391, 0.0902	0.0424, 0.0945	0.0708, 0.1941	0.1577, 0.3872

Residual (e·nm⁻³) 1.178/-2.314 1.086/-2.137 0.873/-2.007 3.534/-2.709 12.377/-7.704

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

Table S2 Anisotropic and isotropic displacement parameters of **1** at selected temperature



	T / K	C (1)	C (2)	C (3)	C (4)	C (5)	N (1)	N (2)
$U_{eq} / \text{\AA}^2$	150	0.023(2)	0.0318(16)	0.0366(18)	0.060(4)	0.056(4)	0.037(2)	0.037(2)
	200	0.033(2)	0.0403(18)	0.047(2)	0.070(5)	0.072(5)	0.048(3)	0.048(3)
	250	0.040(2)	0.049(2)	0.057(2)	0.093(6)	0.089(6)	0.063(3)	0.058(3)
	300	0.047(5)	0.062(4)	0.065(4)	0.073(6)	0.073(7)	0.064(4)	0.072(5)
	350	0.051(10)	0.079(11)	0.080(10)	0.103(18)	0.13(3)	0.090(13)	0.078(11)
$U_{11} / \text{\AA}^2$	150	0.020(5)	0.040(4)	0.043(4)	0.038(7)	0.024(6)	0.038(5)	0.029(5)
	200	0.033(5)	0.051(5)	0.050(5)	0.045(7)	0.033(7)	0.048(6)	0.035(5)

	250	0.040(6)	0.064(5)	0.063(5)	0.066(9)	0.048(9)	0.067(7)	0.044(5)
	300	0.04(2)	0.057(17)	0.068(16)	0.09(3)	0.10(5)	0.07(2)	0.061(19)
	350	0.05(3)	0.08(3)	0.08(2)	0.10(5)	0.13(7)	0.09(3)	0.08(3)
	150	0.027(5)	0.025(3)	0.045(5)	0.123(14)	0.108(13)	0.031(5)	0.066(7)
	200	0.034(5)	0.029(3)	0.053(5)	0.142(15)	0.125(15)	0.039(5)	0.081(8)
$U_{22} / \text{\AA}^2$	250	0.041(5)	0.035(4)	0.061(5)	0.177(19)	0.156(19)	0.045(5)	0.094(8)
	300	0.04(2)	0.057(19)	0.068(19)	0.09(3)	0.10(5)	0.07(2)	0.061(19)
	350	0.05(2)	0.08(3)	0.08(3)	0.10(5)	0.13(7)	0.09(3)	0.08(3)
	150	0.022(5)	0.030(4)	0.022(3)	0.019(5)	0.036(7)	0.043(6)	0.016(4)
	200	0.033(5)	0.040(4)	0.037(4)	0.022(5)	0.057(9)	0.058(6)	0.028(5)
$U_{33} / \text{\AA}^2$	250	0.038(6)	0.049(5)	0.047(5)	0.036(7)	0.062(10)	0.077(8)	0.036(5)
	300	0.045(17)	0.057(14)	0.068(14)	0.09(3)	0.10(4)	0.073(19)	0.061(16)
	350	0.051(19)	0.08(2)	0.080(19)	0.10(3)	0.13(6)	0.09(3)	0.08(2)

Table S3 CIE coordinates of **1** at selected temperature

Temperature (K)	CIE coordinates
300	(0.408, 0.447)
275	(0.425, 0.462)
250	(0.435, 0.471)
225	(0.426, 0.479)
200	(0.380, 0.483)
175	(0.337, 0.476)
150	(0.371, 0.466)

125	(0.436, 0.456)
100	(0.478, 0.441)
85	(0.491, 0.432)
70	(0.512, 0.422)
55	(0.541, 0.412)
40	(0.566, 0.399)
25	(0.581, 0.391)
10	(0.595, 0.384)

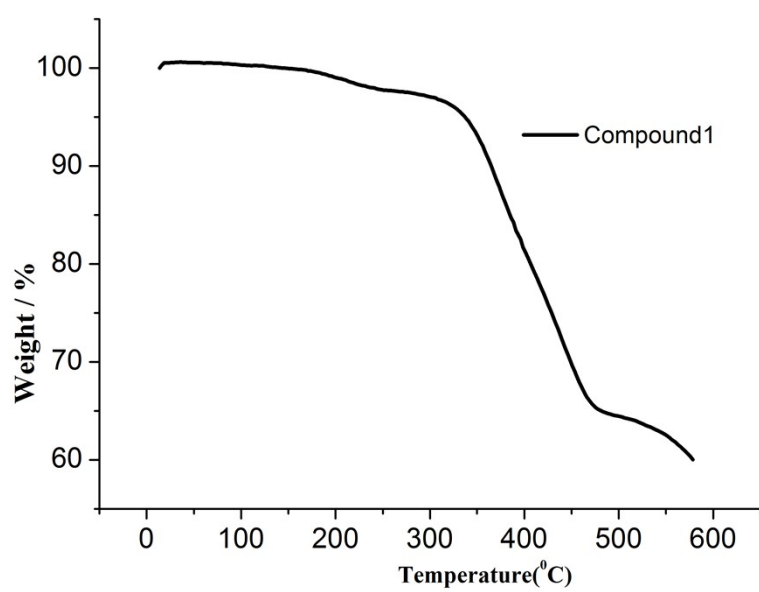


Figure S1 TG curver of 1

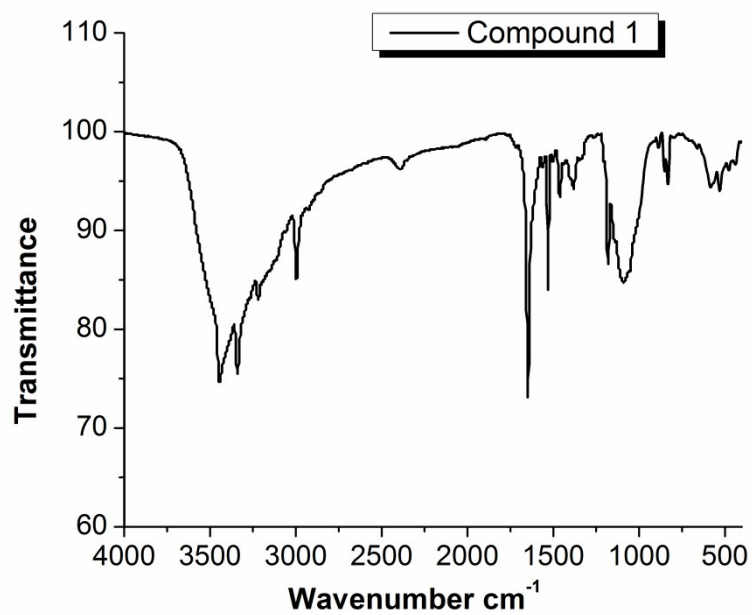


Figure S2 IR curve of **1** at room temperature

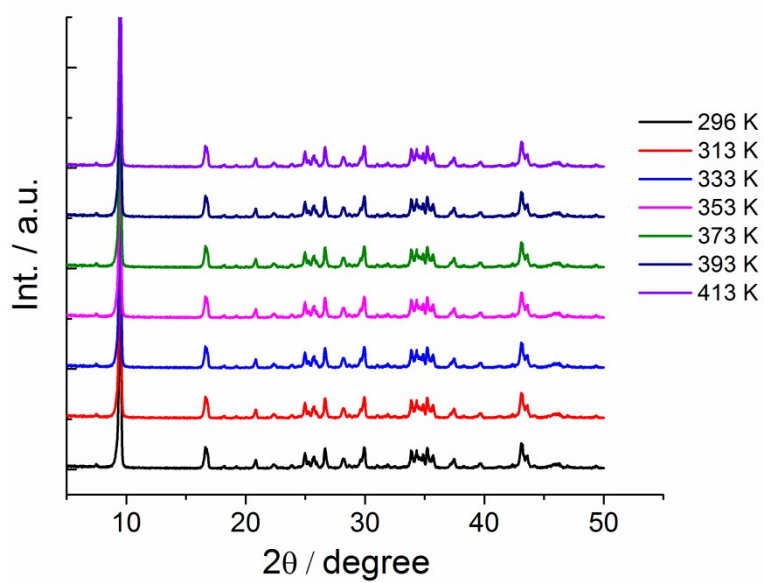


Figure S3 Temperature-dependent PXRD of **1** at 296-413 K

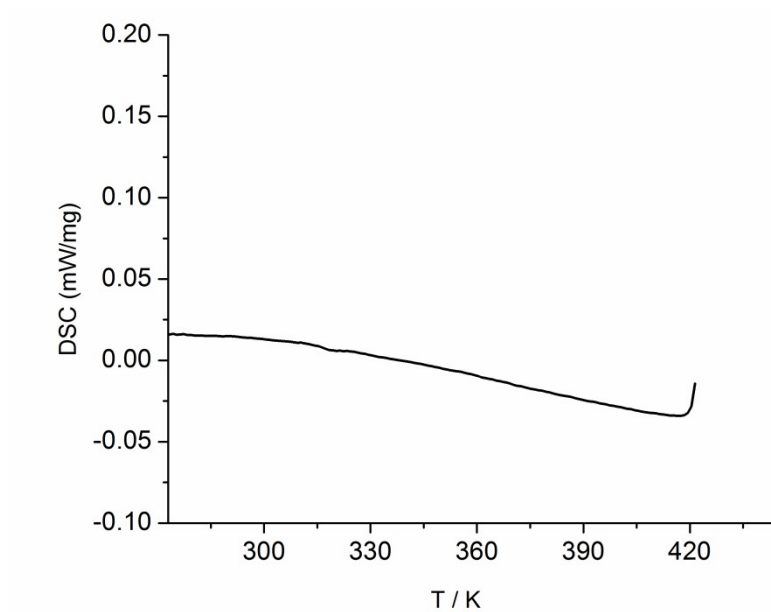


Figure S4 DSC curves of **1** in the heating run at 271-420 K

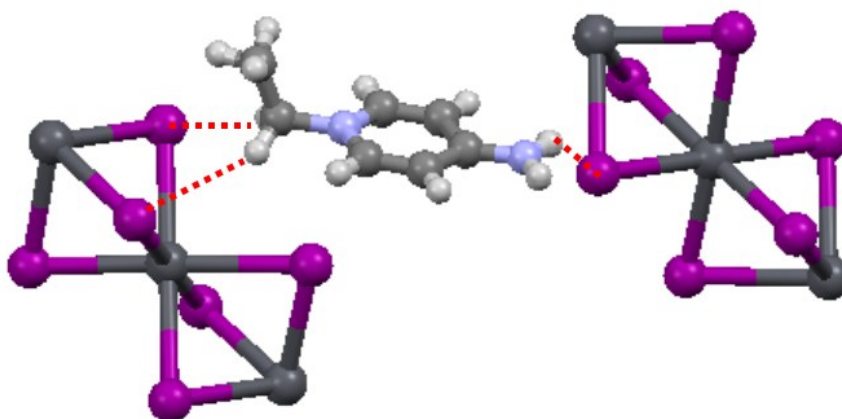


Figure S5 The charge-assisted H-bonding interactions of the cation and the I⁻ anions of the inorganic chain

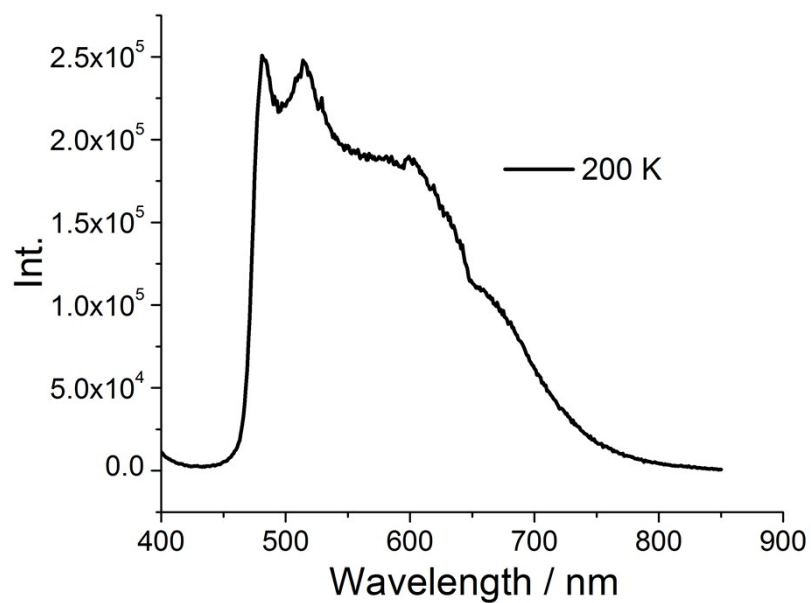


Figure S6 Emission spectra of **1** at 200 K

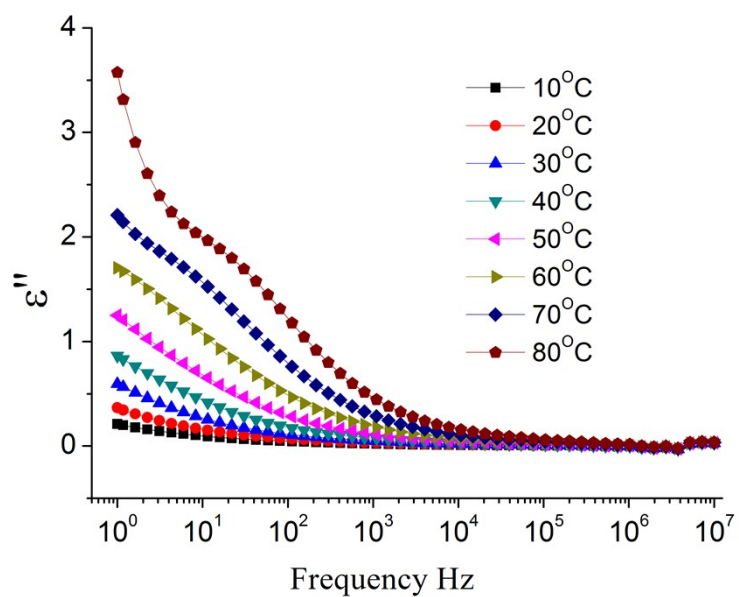


Figure S7 Frequency dependencies of the ϵ'' of **1** in the 10-80 °C temperature range

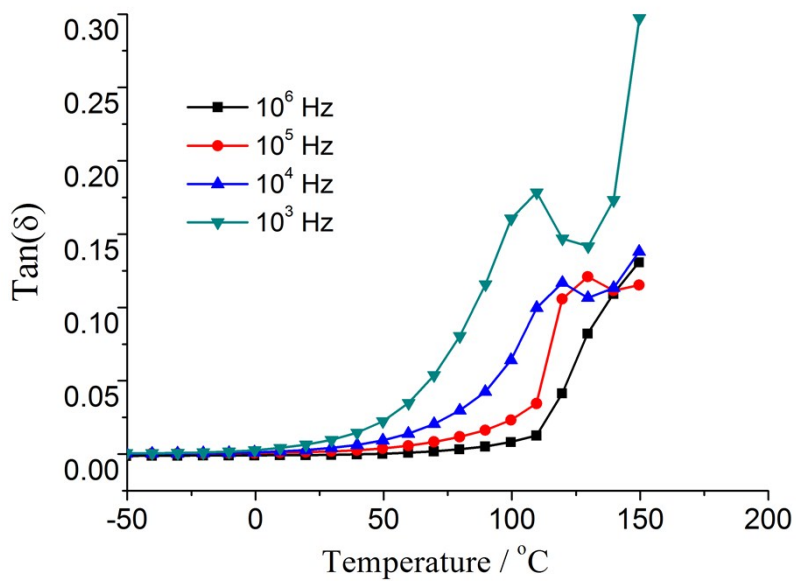


Figure S8 Temperature dependencies of $\tan(\delta)$ of **1** at selected frequency

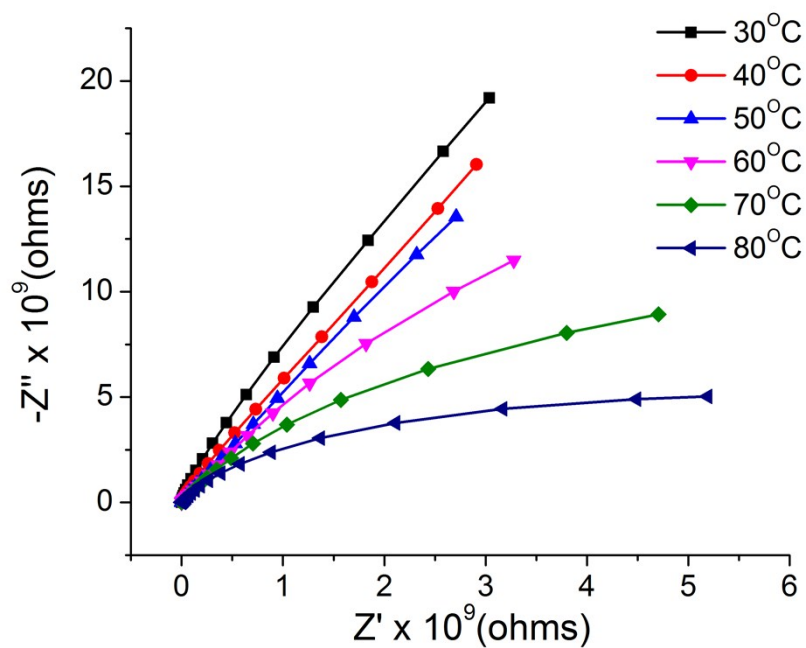


Figure S9 Complex impedance of **1** at selected temperature