Electronic Supplementary Information

Investigation of thermochromic photoluminescent, dielectric and crystal structural properties for an inorganic-organic hybrid solid of [1-hexyl-3-methylimidazolium][$PbBr_3$]

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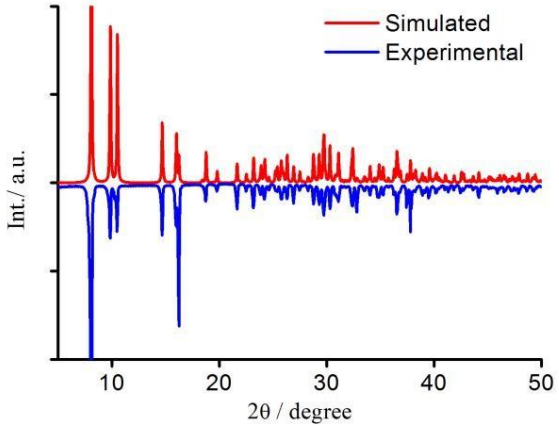


Fig. S1: Powder X-ray diffraction patterns for as-prepared sample of **1**, confirming the phase purity of the as-prepared sample (Blue lines: experimental patterns; red lines: simulated profiles).

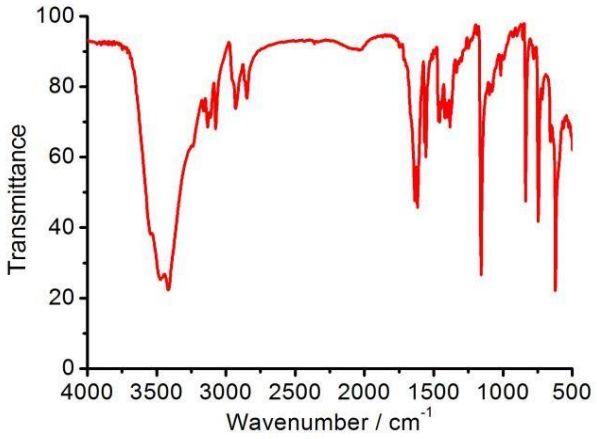


Fig. S2: FT-IR spectra for **1** ($\nu_{C=N}$ = 1622 cm^{-1})

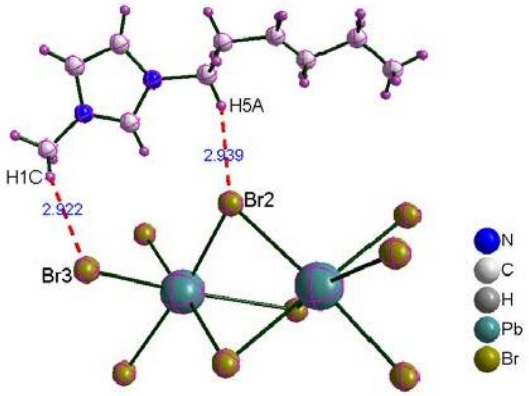


Fig. S3: The weak interaction of C-H…Br between organic cation and inorganic anion for **1** at room temperature.

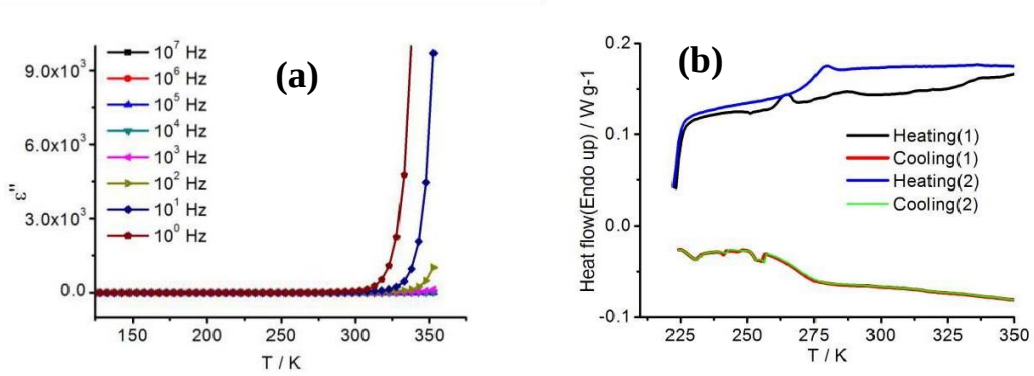
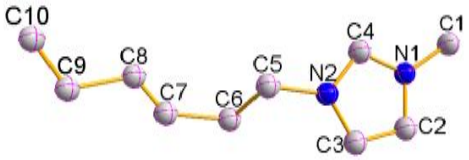


Fig. S4: (a) Plots of imaginary (ε") parts of dielectric permittivity versus temperature in 123-353 K (b) DSC curves with two sequentially heating-cooling runs in 223-353 K for **1**.

Table S1: Parameters of impedance from fits for **1** at selected temperatures.

T / K	333	338	343	348	353
R1 / Ω	7.582×10^{6}	5.056×10^{6}	2.965×10^{6}	1.752×10^{6}	8.961×10^{5}
R2 / Ω	3.383×10^{7}	1.525×10^{7}	6.790×10^{6}	3.094×10^{6}	1.418×10^{6}
σ1 / S cm^{-1}	1.126×10^{-8}	1.688×10^{-8}	2.879×10^{-8}	4.872×10^{-8}	9.525×10^{-8}
σ2 / S cm^{-1}	2.523×10^{-9}	5.597×10^{-9}	1.257×10^{-8}	2.759×10^{-8}	6.019×10^{-8}

Table S2: Atom displacement parameters (U_{eq}, U_{11}, U_{22} and U_{33}) for cations of **1** at 173, 223, 243,263, 283 and 313 K.



Atom	Temp. / K	U_{eq} / Å^2	U_{11} / Å^2	U_{22} / Å^2	U_{33} / Å^2
C1	173	0.047(3)	0.067(7)	0.034(5)	0.057(7)
	223	0.057(4)	0.081(10)	0.040(7)	0.071(10)
	243	0.065(4)	0.093(12)	0.046(8)	0.076(12)
	263	0.067(4)	0.090(11)	0.046(7)	0.087(12)
	283	0.072(5)	0.096(12)	0.052(9)	0.094(13)
	313	0.093(11)	0.12(3)	0.07(2)	0.11(3)
C2	173	0.0297(18)	0.021(4)	0.033(4)	0.039(5)
	223	0.035(3)	0.027(5)	0.033(6)	0.047(7)
	243	0.040(3)	0.030(6)	0.040(7)	0.050(8)
	263	0.046(3)	0.029(5)	0.050(7)	0.059(8)
	283	0.047(3)	0.033(6)	0.053(8)	0.053(8)
	313	0.058(7)	0.041(15)	0.045(13)	0.08(2)
C3	173	0.0265(16)	0.022(4)	0.027(4)	0.035(4)
	223	0.033(2)	0.021(5)	0.046(7)	0.037(6)
	243	0.038(3)	0.025(5)	0.050(7)	0.043(7)
	263	0.043(3)	0.035(6)	0.046(6)	0.050(7)
	283	0.045(3)	0.037(6)	0.049(7)	0.056(8)
	313	0.053(6)	0.028(12)	0.067(15)	0.077(19)
C4	173	0.0290(17)	0.018(3)	0.041(5)	0.031(4)
	223	0.034(2)	0.029(5)	0.039(6)	0.040(6)
	243	0.038(3)	0.033(6)	0.039(6)	0.042(7)
	263	0.041(3)	0.035(5)	0.045(6)	0.052(7)
	283	0.046(3)	0.038(6)	0.048(7)	0.059(8)
	313	0.047(6)	0.052(14)	0.032(11)	0.061(16)
C5	173	0.047(2)	0.056(6)	0.050(6)	0.036(5)
	223	0.053(3)	0.056(8)	0.052(8)	0.049(8)
	243	0.057(4)	0.071(9)	0.049(8)	0.050(8)
	263	0.059(3)	0.064(8)	0.050(8)	0.063(9)
	283	0.064(4)	0.068(9)	0.056(9)	0.071(11)
	313	0.071(8)	0.08(2)	0.053(15)	0.08(2)
C6	173	0.044(2)	0.061(6)	0.043(6)	0.033(5)
	223	0.061(4)	0.082(11)	0.055(9)	0.046(8)
	243	0.074(5)	0.104(14)	0.060(10)	0.055(10)
	263	0.078(5)	0.112(13)	0.054(9)	0.060(10)
	283	0.088(6)	0.131(17)	0.063(11)	0.063(11)

	313	0.101(12)	0.14(4)	0.06(2)	0.09(3)
C7	173	0.145(11)	0.29(3)	0.115(15)	0.057(10)
	223	0.157(15)	0.30(5)	0.092(18)	0.09(2)
	243	0.160(15)	0.29(5)	0.093(19)	0.11(2)
	263	0.168(14)	0.26(4)	0.099(19)	0.13(2)
	283	0.190(17)	0.25(4)	0.13(3)	0.15(3)
	313	0.17(3)	0.23(7)	0.08(3)	0.15(5)
C8	173	0.119(8)	0.24(2)	0.062(9)	0.120(15)
	223	0.153(15)	0.29(4)	0.068(15)	0.17(3)
	243	0.168(17)	0.32(5)	0.081(18)	0.18(3)
	263	0.190(18)	0.31(5)	0.087(18)	0.24(4)
	283	0.24(3)	0.38(6)	0.09(2)	0.34(6)
	313	0.26(5)	0.41(12)	0.05(3)	0.35(11)
C9	173	0.085(5)	0.106(12)	0.098(11)	0.070(9)
	223	0.108(9)	0.126(19)	0.112(18)	0.112(19)
	243	0.118(10)	0.13(2)	0.12(2)	0.12(2)
	263	0.130(10)	0.16(2)	0.124(19)	0.13(2)
	283	0.154(14)	0.20(3)	0.15(3)	0.15(3)
	313	0.20(4)	0.22(7)	0.20(6)	0.26(8)
C10	173	0.097(6)	0.169(19)	0.074(10)	0.069(10)
	223	0.123(10)	0.21(3)	0.090(16)	0.100(19)
	243	0.127(11)	0.21(3)	0.106(18)	0.082(17)
	263	0.153(12)	0.26(4)	0.098(17)	0.14(2)
	283	0.159(13)	0.26(4)	0.12(2)	0.13(3)
	313	0.18(3)	0.26(8)	0.16(5)	0.14(5)
N1	173	0.0259(14)	0.027(3)	0.025(3)	0.032(4)
	223	0.031(2)	0.031(5)	0.030(5)	0.039(5)
	243	0.034(2)	0.034(5)	0.033(5)	0.041(6)
	263	0.037(2)	0.035(5)	0.042(5)	0.039(5)
	283	0.040(2)	0.037(5)	0.041(6)	0.046(6)
	313	0.046(5)	0.040(12)	0.044(11)	0.061(14)
N2	173	0.0285(15)	0.027(3)	0.036(4)	0.024(3)
	223	0.032(2)	0.031(5)	0.030(5)	0.034(5)
	243	0.037(2)	0.037(5)	0.036(5)	0.040(6)
	263	0.038(2)	0.037(5)	0.039(5)	0.040(5)
	283	0.043(2)	0.046(6)	0.039(5)	0.042(6)
	313	0.048(5)	0.049(12)	0.034(9)	0.062(14)
Pb1	173	0.01914(10)	0.02582(16)	0.01415(16)	0.02287(16)
	223	0.02328(15)	0.0279(2)	0.0174(2)	0.0282(2)
	243	0.02575(15)	0.0302(2)	0.0193(2)	0.0315(3)
	263	0.02757(14)	0.0308(2)	0.02115(19)	0.0345(2)
	283	0.03007(15)	0.0335(2)	0.0226(2)	0.0381(3)
	313	0.0330(4)	0.0366(6)	0.0230(4)	0.0432(6)
Br1	173	0.02507(18)	0.0273(4)	0.0338(4)	0.0183(4)

	223	0.0320(3)	0.0357(6)	0.0408(6)	0.0225(5)
	243	0.0356(3)	0.0394(6)	0.0450(7)	0.0251(6)
	263	0.0379(3)	0.0414(6)	0.0477(6)	0.0268(5)
	283	0.0415(3)	0.0465(6)	0.0506(7)	0.0304(6)
	313	0.0458(6)	0.0514(15)	0.0536(13)	0.0352(13)
Br2	173	0.03000(19)	0.0287(4)	0.0262(4)	0.0326(4)
	223	0.0369(3)	0.0313(6)	0.0307(6)	0.0428(7)
	243	0.0403(3)	0.0338(6)	0.0330(6)	0.0477(7)
	263	0.0433(3)	0.0346(6)	0.0369(6)	0.0511(7)
	283	0.0468(3)	0.0373(6)	0.0396(6)	0.0557(8)
	313	0.0519(7)	0.0400(14)	0.0402(12)	0.0676(18)
Br3	173	0.02844(19)	0.0422(4)	0.0202(4)	0.0374(4)
	223	0.0359(3)	0.0484(6)	0.0266(5)	0.0475(7)
	243	0.0398(3)	0.0523(7)	0.0300(6)	0.0531(8)
	263	0.0425(3)	0.0546(7)	0.0329(5)	0.0563(7)
	283	0.0458(3)	0.0582(7)	0.0357(6)	0.0610(8)
	313	0.0518(7)	0.0637(16)	0.0356(11)	0.0757(19)

Table S3: CIE chromaticity of **1** at different temperatures

T / K	CIE x	CIE y	Peak center location(nm) (compound light)	Relative intensity
10	0.2616	0.1799	452	2874210
25	0.3082	0.21	454	1825780
40	0.3594	0.2419	667	1402310
55	0.418	0.2823	636	1441270
70	0.4728	0.3212	640	1495400
85	0.5021	0.3455	635	1270380
100	0.5165	0.3622	632	1077250
115	0.5216	0.3718	635	755367
140	0.5228	0.38	628	449142
165	0.5163	0.3926	626	285068
190	0.5067	0.4017	620	198835
215	0.4936	0.4074	620	128919
240	0.4789	0.4096	623	78879
265	0.4668	0.4069	615	51912
300	0.4444	0.4024	613	27000

Table S4: Intensity and intensity ratio of emission bands in selected temperatures for **1**.

T / K	Peak 1 intensity (I_{T1})	Peak 2 intensity (I_{T2})	I_{T1} / $I_{300(1)}$	I_{T2} / $I_{300(2)}$	I_{T1}/I_{T2}
10	2.86E+06	1.21E+06	388.9300747	45.46902522	2.36099
25	1.81E+06	1.32E+06	246.4317719	49.42735075	1.37616
40	1.23E+06	1.40E+06	166.8553971	52.49522168	0.87732
55	777898	1.44E+06	105.6209097	53.93284113	0.54055
70	463928	1.49E+06	62.99090292	55.83517595	0.31139
85	267345	1.27E+06	36.299389	47.54637784	0.21073
100	172564	1.07E+06	23.43027834	40.06521006	0.16142
115	102667	754455	13.93985064	28.27474422	0.13608
140	55183	446086	7.492600136	16.71798523	0.1237
165	33774	280595	4.585743381	10.51587153	0.12037
190	25206	198527	3.422403259	7.440205374	0.12697
215	19160	128595	2.601493551	4.819360642	0.14899
240	13784	78255	1.87155465	2.932766181	0.17614
265	10633	50173	1.443720299	1.880335794	0.21193
300	7365	26683	1	1	0.27602

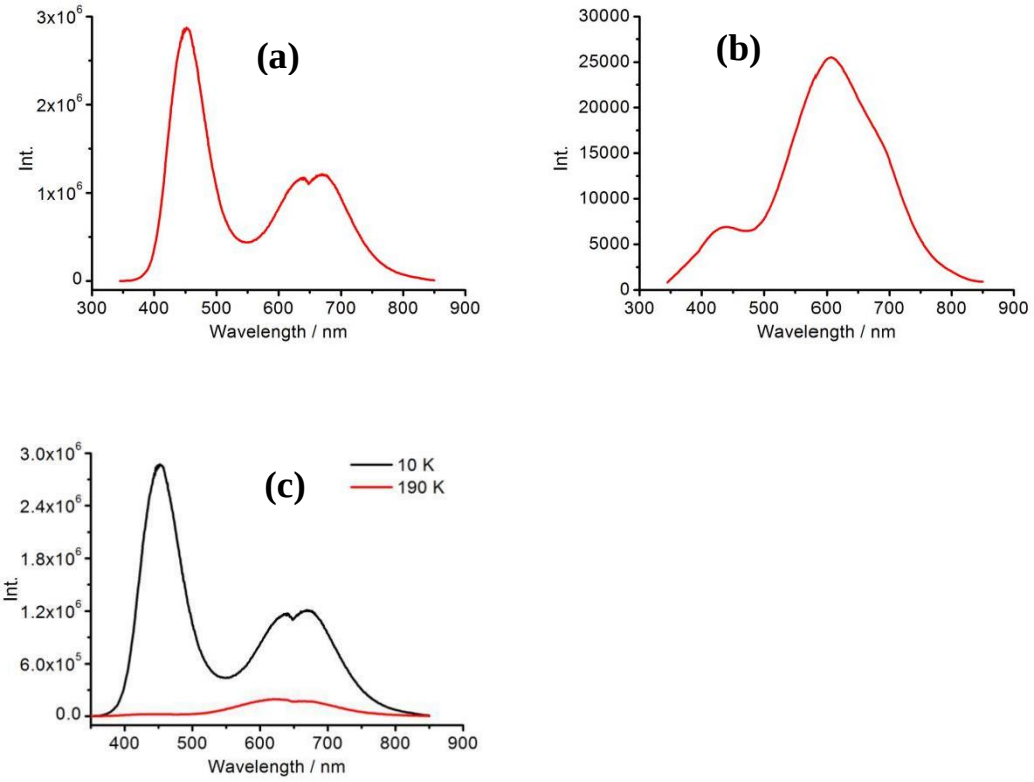


Fig. S5: PL spectrum (a) at 10 K (b) at 300 K and (c) comparison between 10 and 190

K with λ_{ex} = 325 nm for **1**.

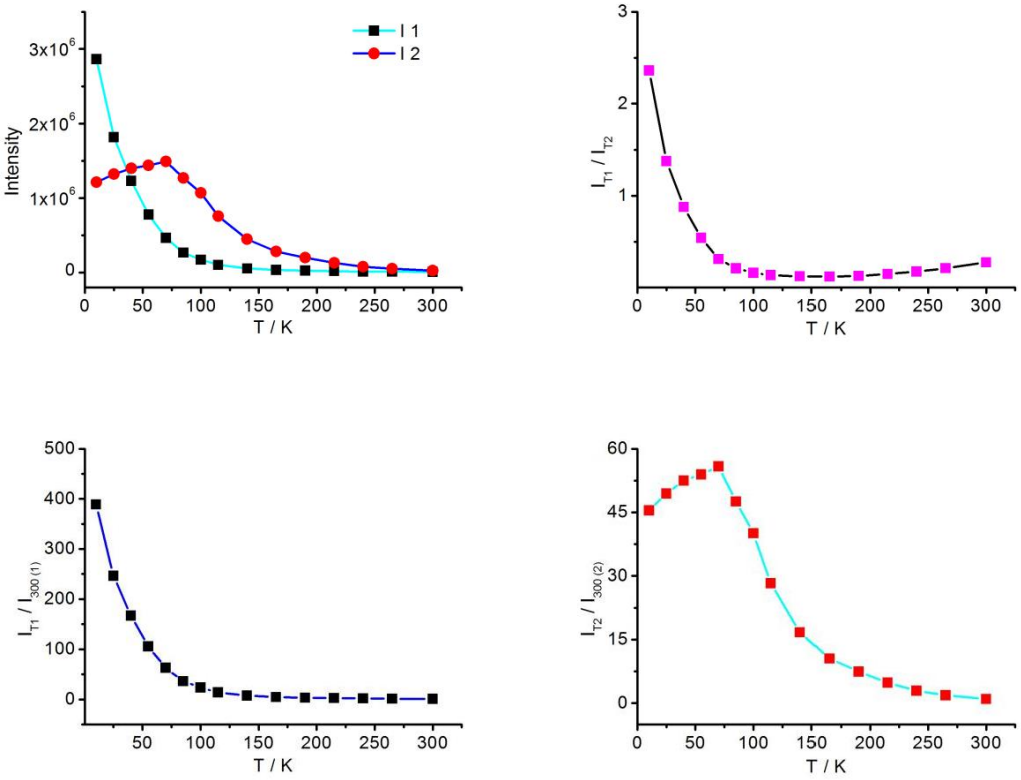


Fig.S6: (a) Peak intensity and (b) peak intensity ratio at selected temperatures (c, d) the ratio of peak intensity at selected temperatures towards the peak intensity of 300 K for every emission band.