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Reversible solid-state thermochromism of a 2D organic-inorganic hybrid perovskite structure based on iodoplumbate and 2-aminomethyl-pyridine

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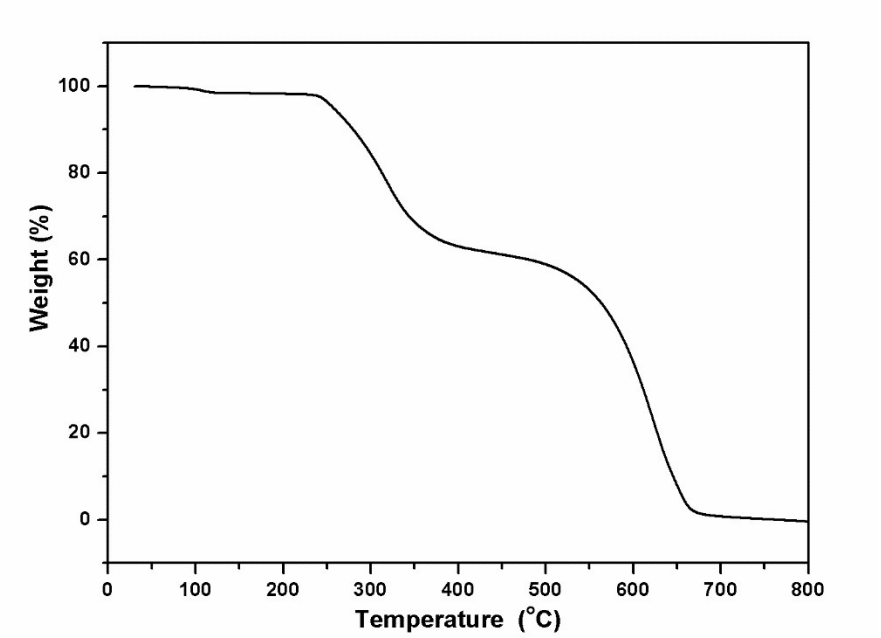

Figure 1s TG curve of compound **1**.

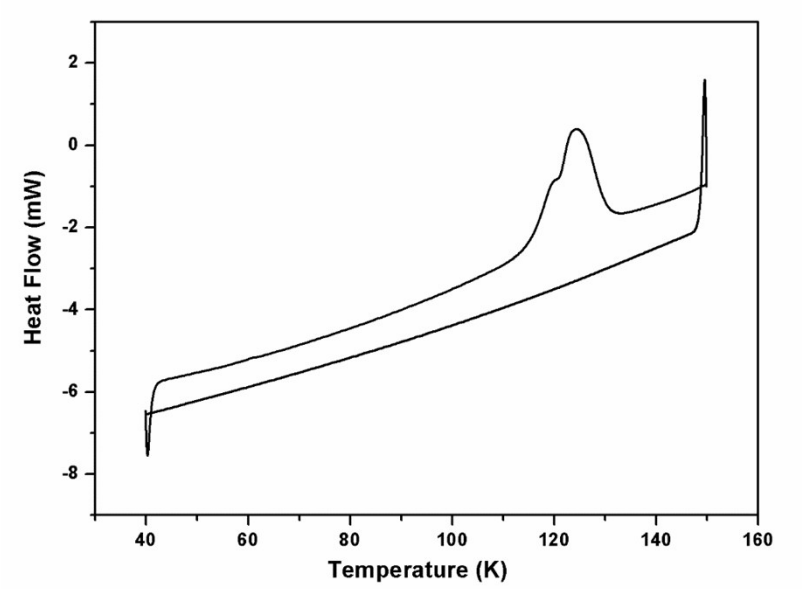

Figure 2s the DSC curve of compound **1**.

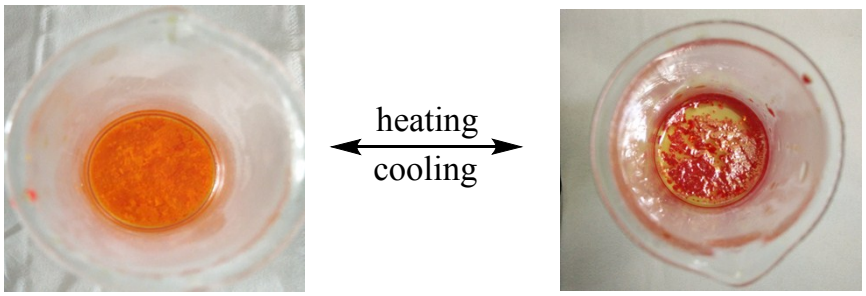

Figure 3s the thermochromism of **1** occurred in the HI solution

Table 1s Crystallographic data for complex **1**

Complex	**1**
Empirical formula	$C_{36}H_{60}I_{22}N_{12}O_3Pb_5$
Formula weight	4536.76
Temperature	293(2) K

Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, *Pnma*
Unit cell dimensions	a = 26.628(6) Å α = 90° b = 12.917(3) Å β = 90° c = 26.346(6) Å γ = 90°
Volume	9062(4) Å^3
Z, Calculated density	4, 3.325 Mg/cm^3
Absorption coefficient	16.789 mm^{-1}
F(000)	7840
Crystal size	0.20 × 0.18 × 0.05 mm
Theta range for data collection	2.89 to 25.00°
Limiting indices	-31<=h<=31 -15<=k<=12 -31<=l<=20
Reflections collected / unique	41820 / 8168 [R(int) = 0.0381]
Completeness to theta	97.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.432 and 0.049
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8168 / 0 / 388
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R_1 = 0.0381, wR_2 = 0.1119

R indices (all data)	$R_1 = 0.0525$, $wR_2 = 0.1326$
Largest diff. peak and hole	1.754 and −3.183 e. Å^{-3}

Table 2s the selected bonds and angles in complex **1**

Pb(1)-I(1)	3.0470(15)	Pb(1)-I(3)#1	3.1863(11)
Pb(1)-I(3)	3.1863(11)	Pb(1)-I(2)	3.1912(14)
Pb(1)-I(5)	3.2585(14)	Pb(1)-I(4)	3.4096(14)
Pb(2)-I(5)	3.1851(14)	Pb(2)-I(7)	3.2203(14)
Pb(2)-I(8)#1	3.2258(11)	Pb(2)-I(8)	3.2258(11)
Pb(2)-I(6)	3.2294(15)	Pb(2)-I(4)	3.3035(15)
Pb(3)-I(10)	3.0931(15)	Pb(3)-I(9)	3.1407(14)
Pb(3)-I(12)	3.1990(14)	Pb(3)-I(8)	3.2516(11)
Pb(3)-I(8)#2	3.2516(11)	Pb(3)-I(11)	3.3176(14)
Pb(4)-I(14)	3.0090(15)	Pb(4)-I(15)	3.1905(14)
Pb(4)-I(13)	3.2216(16)	Pb(4)-I(16)	3.2425(11)
Pb(4)-I(16)#2	3.2425(11)	Pb(5)-I(18)	3.0008(14)
Pb(5)-I(17)	3.0144(15)	Pb(5)-I(16)#1	3.2471(11)
Pb(5)-I(16)	3.2471(11)	I(1)-Pb(1)-I(3)#1	87.22(2)
I(1)-Pb(1)-I(3)	87.22(2)	I(3)#1-Pb(1)-I(3)	174.43(4)
I(1)-Pb(1)-I(2)	96.05(5)	I(3)#1-Pb(1)-I(2)	90.19(2)

I(3)-Pb(1)-I(2)	90.19(2)	I(1)-Pb(1)-I(5)	93.59(4)
I(3)#1-Pb(1)-I(5)	90.27(2)	I(3)-Pb(1)-I(5)	90.28(2)
I(2)-Pb(1)-I(5)	170.36(4)	I(1)-Pb(1)-I(4)	173.40(4)
I(3)#1-Pb(1)-I(4)	92.78(2)	I(3)-Pb(1)-I(4)	92.78(2)
I(2)-Pb(1)-I(4)	90.55(4)	I(5)-Pb(1)-I(4)	79.81(3)
I(5)-Pb(2)-I(7)	85.14(4)	I(5)-Pb(2)-I(8)#1	91.52(2)
I(7)-Pb(2)-I(8)#1	86.40(2)	I(5)-Pb(2)-I(8)	91.52(2)
I(7)-Pb(2)-I(8)	86.40(2)	I(8)#1-Pb(2)-I(8)	171.92(4)
I(5)-Pb(2)-I(6)	172.82(4)	I(7)-Pb(2)-I(6)	102.03(4)
I(8)#1-Pb(2)-I(6)	88.96(2)	I(8)-Pb(2)-I(6)	88.96(2)
I(5)-Pb(2)-I(4)	82.50(4)	I(7)-Pb(2)-I(4)	167.65(4)
I(8)#1-Pb(2)-I(4)	93.908(19)	I(8)-Pb(2)-I(4)	93.908(19)
I(6)-Pb(2)-I(4)	90.32(4)	I(10)-Pb(3)-I(9)	95.87(4)
I(10)-Pb(3)-I(12)	174.94(4)	I(9)-Pb(3)-I(12)	89.19(4)
I(10)-Pb(3)-I(8)	94.404(19)	I(9)-Pb(3)-I(8)	87.93(2)
I(12)-Pb(3)-I(8)	85.758(19)	I(10)-Pb(3)-I(8)#2	94.404(19)
I(9)-Pb(3)-I(8)#2	87.93(2)	I(12)-Pb(3)-I(8)#2	85.758(19)
I(8)-Pb(3)-I(8)#2	170.60(4)	I(10)-Pb(3)-I(11)	92.22(4)
I(9)-Pb(3)-I(11)	171.91(4)	I(12)-Pb(3)-I(11)	82.72(3)
I(8)-Pb(3)-I(11)	91.46(2)	I(8)#2-Pb(3)-I(11)	91.46(2)
I(14)-Pb(4)-I(15)	89.68(4)	I(14)-Pb(4)-I(13)	88.29(4)
I(15)-Pb(4)-I(13)	177.96(4)	I(14)-Pb(4)-I(16)	96.31(2)

I(15)-Pb(4)-I(16)	88.30(2)	I(13)-Pb(4)-I(16)	91.92(2)
I(14)-Pb(4)-I(16)#2	96.31(2)	I(15)-Pb(4)-I(16)#2	88.30(2)
I(13)-Pb(4)-I(16)#2	91.92(2)	I(16)-Pb(4)-I(16)#2	166.90(4)
I(18)-Pb(5)-I(17)	91.92(4)	I(18)-Pb(5)-I(16)#1	93.31(2)
I(17)-Pb(5)-I(16)#1	92.92(2)	I(18)-Pb(5)-I(16)	93.31(2)
I(17)-Pb(5)-I(16)	92.92(2)	I(16)#1-Pb(5)-I(16)	171.02(4)

Table 3s the hydrogen bonds in compound **1**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (°)
N1-H1C···I3	0.89	2.96	3.635(11)	134
N1H1D···I12	0.89	2.80	3.562(12)	145
N1-H1E···O1	0.89	2.12	3.007(16)	173
N2-H2···O1	0.86	2.14	2.962(18)	160
N3-H3A···I3	0.89	2.99	3.753(13)	145
N3-H3B···I8	0.89	2.89	3.763(12)	165
N3-H3C···I19	0.89	2.78	3.556(13)	146
N4-H4A···I15	0.86	2.64	3.475(12)	163
N5-H5A···I7	0.89	2.80	3.651(15)	159
N5-H5B···I16	0.89	2.82	3.621(12)	150
N5-H5C···I3	0.89	2.78	3.636(13)	162

N6-H6A···O2	0.86	2.05	2.863(13)	158