Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Photoluminescent-dielectric duple switch in a perovskite-type high-temperature phase transition compound: $[(CH_3)_3PCH_2OCH_3][PbBr_3]$

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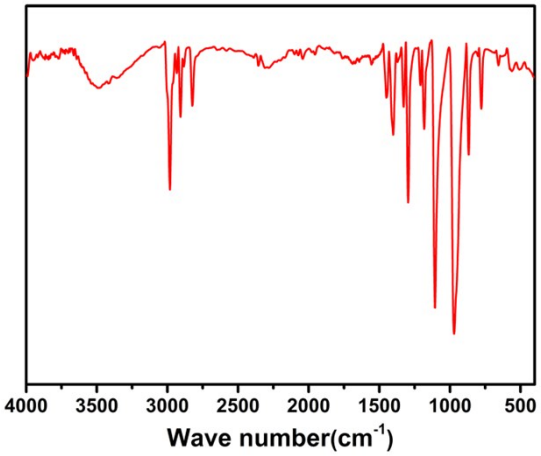

Figure S1. The IR spectrum of compound **1**.

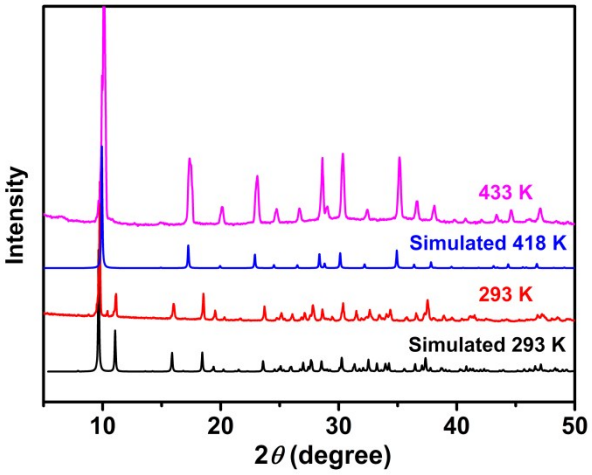

Figure S2. The variable-temperature powder XRD measurement results of compound **1**.

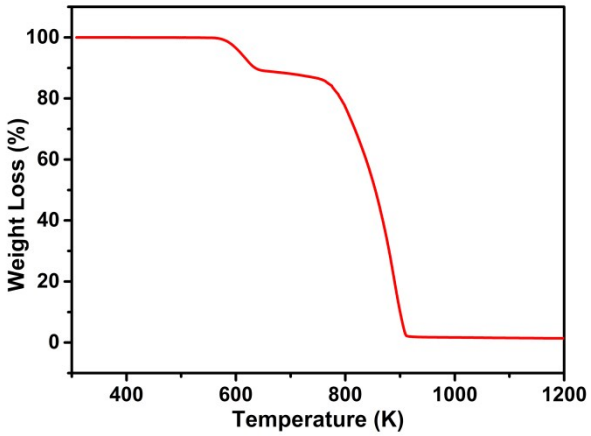

Figure S3. TGA curves of compound **1**.

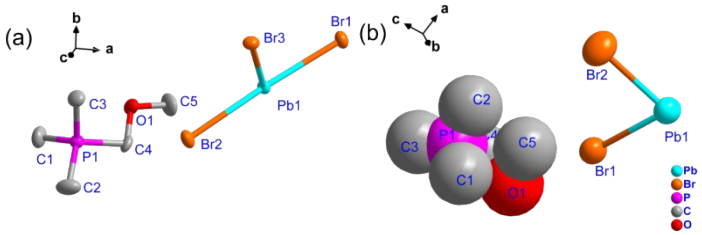

Figure S4. The asymmetric unit of **1** at 293 K(a) and 418 K(b). Thermal ellipsoids for all atoms are shown at the 30% probability level. Hydrogen atoms are omitted for clarity.

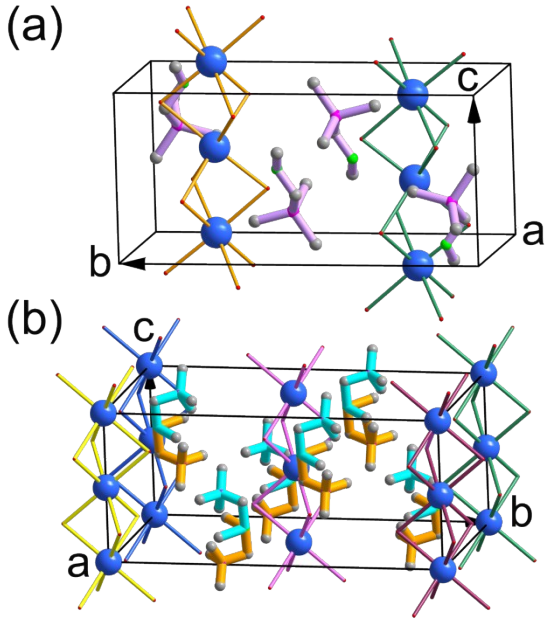

Figure S5. Packing structures in one unit cell of **1** depicted at 293 K(a) and at 418 K(b).

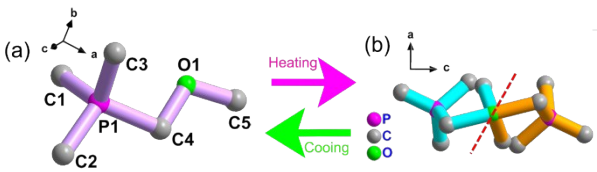

Figure S6.The comparisons of cation of **1** at 293 K(a) and 418 K(b). All hydrogen atoms are omitted for clarity.

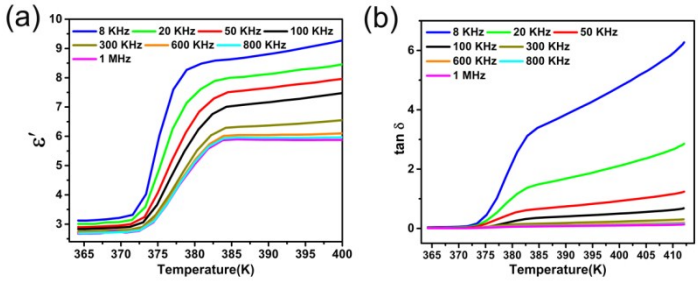

Figure S7. The dielectric constant (ε') and dielectric loss (tan δ) of compound **1** under different frequencies upon cooling.

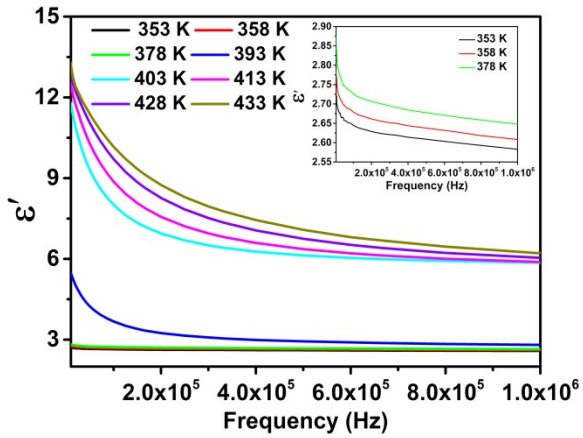

Figure S8. Frequency dependence of the real parts of the dielectric permittivity of **1** obtained at various temperatures.

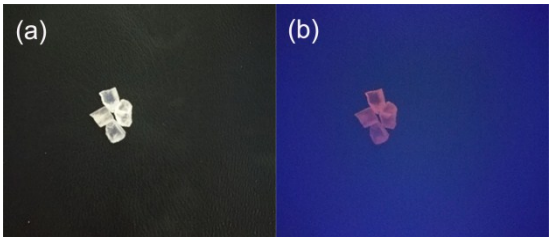

Figure S9. Crystals of **1** under ambient light (a) and under UV light (b).

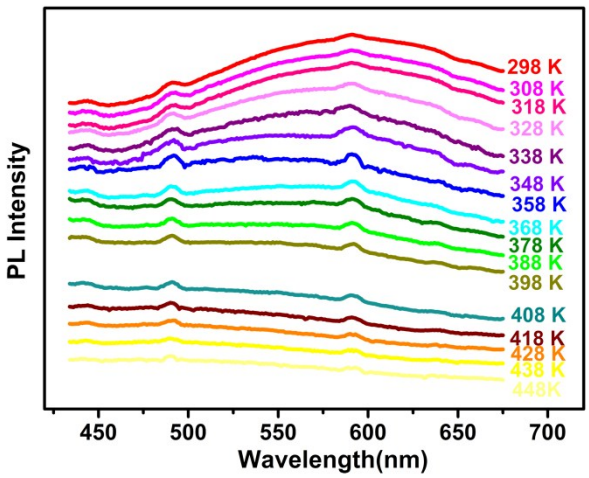

Figure S10. Variable-temperature emission spectra of **1** under 360 nm excitation.

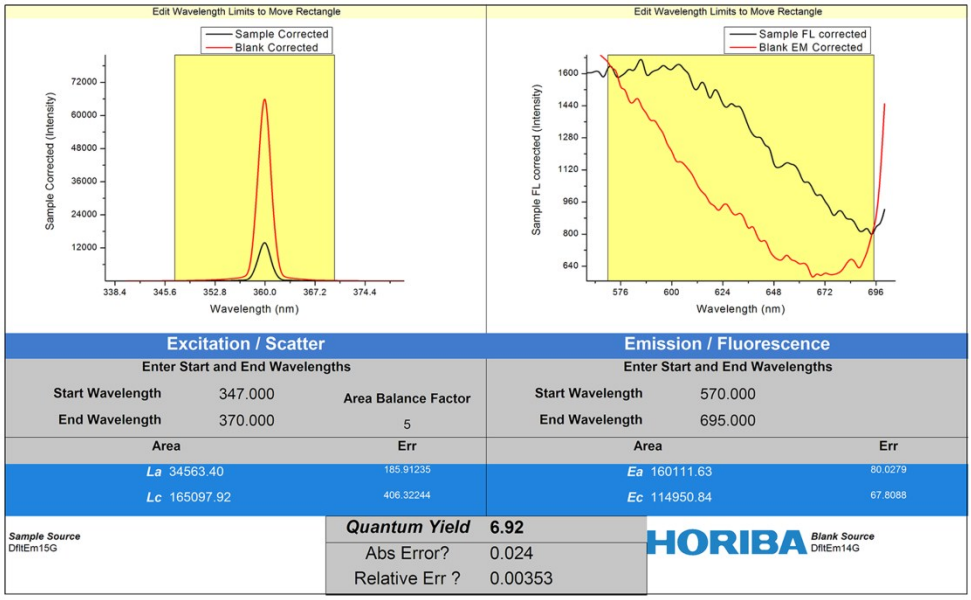

Figure S11. The quantum yield measurement of compound **1.**

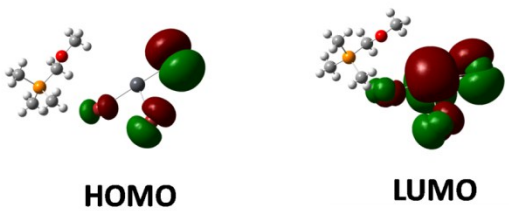

Figure S12. HOMO-LUMO plots of compound **1** at LTP.

Table S1. Crystal data and structure refinements of compound **1**at 293 K and 418 K.

	RTP (293 K)	HTP (418 K)
Chemical formula	$C_5H_{14}OP\ PbBr_3$	$C_5OP\ PbBr_3$
Formula weight	568.03	553.94
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$C2/c$
a, Å	11.240(2)	10.27(3)
b, Å	15.986(3)	17.79(5)
c, Å	7.7734(16)	7.95(2)
β, (°)	97.15(3)	90.0340(12)
V, Å^3	1385.9(5)	1453(7)
Z	4	4
GOF	1.097	1.713
*R*1 [$I > 2\sigma(I)$]	0.0526	0.2261
*WR*2 [$I > 2\sigma(I)$]	0.1002	0.5998

Table S2. The key bond lengths (Å) and bond angels (°) of compound **1** at 293 K and 418 K.

		293 K	418 K
Bond lengths (Å)	Pb1–Br1	3.0364(15)	3.0339(67)
	Pb1–Br2	3.0840(15)	3.0710(81)
	Pb1–Br3	2.9597(13)	
	P1–C1	1.7505(126)	1.3819(75)
	P1–C2	1.7589(144)	1.3683(87)
	P1–C3	1.7609(116)	1.2711(65)
	P1–C4	1.7972(128)	1.3829(71)
	C4–O1	1.4091(145)	1.5171(43)
	O1–C5	1.4126(187)	1.5081(62)
Bond angles (°)	C1–P1–C2	109.875(689)	106.293(493)
	C1–P1–C3	111.609(638)	112.481(340)
	C1–P1–C4	108.291(579)	105.477(439)
	C2–P1–C3	109.079(622)	113.338(456)
	C2–P1–C4	109.707(650)	106.300(405)
	C3–P1–C4	108.247(571)	112.365(403)
	P1–C4–O1	106.677(791)	98.525(243)
	C4–O1–C5	112.789(960)	93.405(153)
	Br1 –Pb1–Br2	85.755(36)	82.085(95)
	Br1 –Pb1–Br3	95.399(36)	
	Br2 –Pb1–Br3	177.225(37)	

Table S3. Equivalent isotropic displacement parameters (U_{iso}) for **1** at 293 K and 418 K.

	293 K	418 K
Atom	Uiso (Å^2)	Uiso (Å^2)
Pb1	0.03118(16)	0.1433(8)
Br1	0.0493(4)	0.1433(8)
Br2	0.0490(3)	0.201(3)
Br3	0.0422(3)	
P1	0.0390(7)	0.725(3)
C1	0.071(4)	0.720(3)
C2	0.086(5)	0.721(3)
C3	0.056(4)	0.719(6)
C4	0.045(3)	0.743(3)
C5	0.078(5)	0.749(3)
O1	0.059(2)	0.754(3)