

Supporting Information

Temperature-Responsive Emission and Elastic Properties of a New 2D

Lead Halide Perovskite

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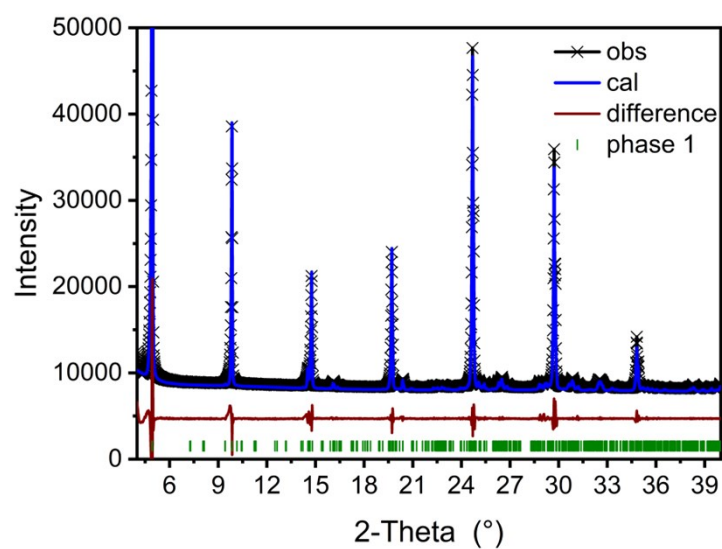


Fig. S1 The powder X-ray diffraction spectra of $(\text{C}_9\text{H}_{14}\text{ON})_2\text{PbI}_4$ refined using the Le-Bail method at ambient conditions. The black, blue symbol and red continuous line are experimental, calculated and difference profiles, respectively, and the vertical green markers indicate the allowed Bragg reflections.

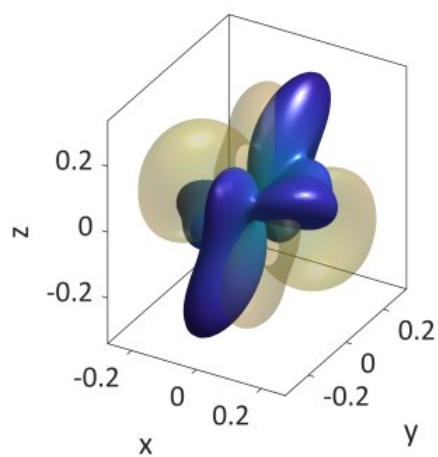


Fig. S2 3D representation of Poisson's ratios of $(\text{C}_9\text{H}_{14}\text{ON})_2\text{PbI}_4$.

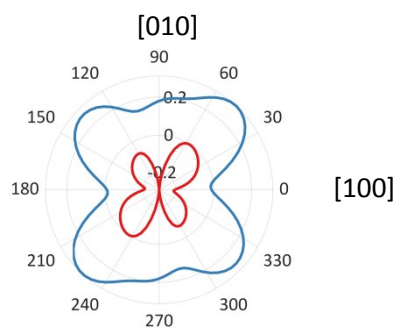


Fig. S3 2D representation of Poisson's ratios of $(\text{C}_9\text{H}_{14}\text{ON})_2\text{PbI}_4$.

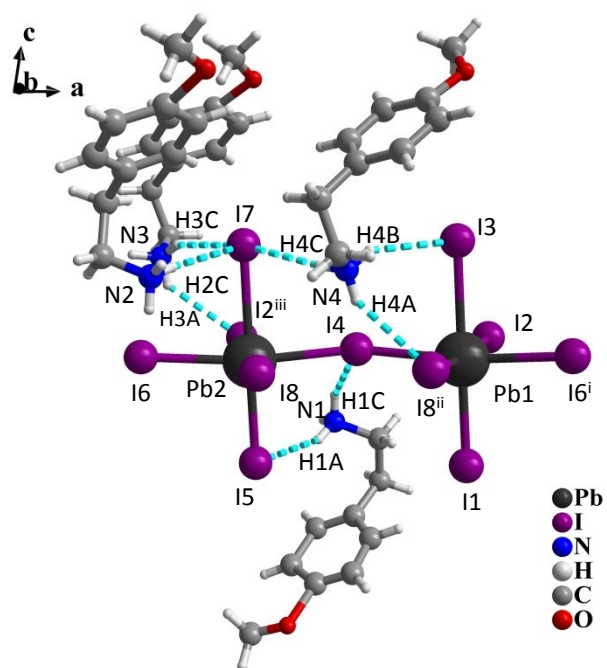


Fig. S4 The crystal structure of $(\text{C}_9\text{H}_{14}\text{ON})_2\text{PbI}_4$. Symmetry codes: i $1 + x, + y, + z$; ii $1 - x, - y, 1 - z$; iii $1 - x, 1 - y, 1 - z$.

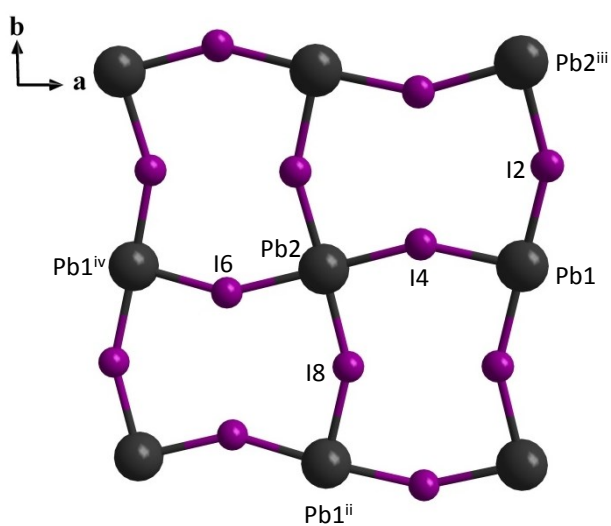


Fig. S5 The inorganic unit of $(\text{C}_9\text{H}_{14}\text{ON})_2\text{PbI}_4$. Symmetry codes: i $1 + X, + Y, + Z$; ii $1 - X, - Y, 1 - Z$; iii $1 - X, 1 - Y, 1 - Z$; iv $-1 + X, + Y, + Z$.

Table S1 Crystal data and structure refinement for (C₉H₁₄ON)₂PbI₄.

Formula	C ₁₈ H ₂₈ I ₄ N ₂ O ₂ Pb
M_w	1019.21
T/K	223
Crystal system	triclinic
Space group	<i>P</i> -1
$a/\text{\AA}$	12.2659(2)
$b/\text{\AA}$	12.3518(2)
$c/\text{\AA}$	18.4045(2)
$a/^\circ$	80.4430(10)
$b/^\circ$	81.1380(10)
$c/^\circ$	89.9950(10)
$V/\text{\AA}^3$	2715.94(7)
Z	4
$\rho_{\text{calc}}/(\text{g}/\text{cm}^3)$	2.493
μ/mm^{-1}	47.894
$F(000)$	1840.0
GOF	1.039
$R_1^a[I >2s(I)]$	$R_1=0.0610$
	$wR_2=0.1746$
$wR_2^b[\text{all data}]$	$R_1=0.0679$
	$wR_2=0.1822$

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

Table S2 Bond Lengths for (C₉H₁₄ON)₂PbI₄. Symmetry codes: i 1 + x, + y, + z; ii 1 – x, - y, 1 - z; iii 1 - x, 1 - y, 1 - z.

Bond	Length/Å	Bond	Length/Å
Pb1-I2	3.1692(5)	Pb2-I8	3.1758(5)
Pb1-I4	3.1628(6)	Pb2-I5	3.0771(6)
Pb1-I6 ⁱ	3.1712(5)	N1-H1A...I5	3.6362(82)
Pb1-I8 ⁱⁱ	3.1985(5)	N1-H1C...I4	3.6340(71)
Pb1-I3	3.4015(7)	N2-H2C...I7	3.6745(82)
Pb1-I1	3.0745(7)	N3-H3A...I2 ⁱⁱⁱ	3.6523(65)
Pb2-I2 ⁱⁱⁱ	3.1916(5)	N3-H3C...I7	3.6948(70)
Pb2-I4	3.1719(6)	N4-H4A...I8 ⁱⁱ	3.6298(69)
Pb2-I6	3.1625(6)	N4-H4B...I3	3.6996(74)
Pb2-I7	3.3996(6)	N4-H4C...I7	3.6994(71)

Table S3 Bond Angles for (C₉H₁₄ON)₂PbI₄. Symmetry codes: i 1 + X, + Y, + Z; ii 1 - X, - Y, 1 - Z; iii 1 - X, 1 - Y, 1 - Z; iv -1 + X, + Y, + Z.

Bond Angles	Angle/°	Bond Angles	Angle/°
I2-Pb1-I6 ⁱ	90.963(15)	I6-Pb2-I7	84.386(16)
I2-Pb1-I8 ⁱⁱ	172.845(19)	I6-Pb2-I8	89.921(15)
I2-Pb1-I3	85.581(16)	I8-Pb2-I2 ⁱⁱⁱ	172.734(18)
I4-Pb1-I2	90.489(15)	I8-Pb2-I7	85.510(15)
I4-Pb1-I6 ⁱ	172.347(19)	I5-Pb2-I2 ⁱⁱⁱ	91.937(16)
I4-Pb1-I8 ⁱⁱ	89.200(15)	I5-Pb2-I4	91.893(17)
I4-Pb1-I3	84.827(16)	I5-Pb2-I6	96.017(18)
I6 ⁱ -Pb1-I8 ⁱⁱ	88.424(15)	I5-Pb2-I7	179.083(14)
I6 ⁱ -Pb1-I3	87.793(16)	I5-Pb2-I8	95.310(17)
I8 ⁱⁱ -Pb1-I3	87.271(15)	N1-H1A...I5	156.017(501)
I1-Pb1-I2	95.035(17)	N1-H1C...I4	140.385(471)
I1-Pb1-I4	95.597(18)	N2-H2C...I7	171.798(500)
I1-Pb1-I6 ⁱ	91.760(17)	N3-H3A...I2 ⁱⁱⁱ	139.070(463)
I1-Pb1-I8 ⁱⁱ	92.109(17)	N3-H3C...I7	154.53(45)
I1-Pb1-I3	179.246(14)	N4-H4A...I8 ⁱⁱ	142.376(464)
I2 ⁱⁱⁱ -Pb2-I7	87.247(15)	N4-H4B...I3	150.695(449)
I4-Pb2-I2 ⁱⁱⁱ	88.935(15)	N4-H4C...I7	172.264(459)
I4-Pb2-I7	87.676(16)	Pb1-I2-Pb2 ⁱⁱⁱ	152.36(2)
I4-Pb2-I8	91.333(15)	Pb1-I4-Pb2	151.30(2)
I6-Pb2-I2 ⁱⁱⁱ	88.808(15)	Pb2-I6-Pb1 ^{iv}	150.883(19)
I6-Pb2-I4	171.842(19)	Pb2-I8-Pb1 ⁱⁱ	153.22(2)