

Electronic Supplementary Information ESI for:

## Chirality Control in White-Light Emitting 2D Perovskites

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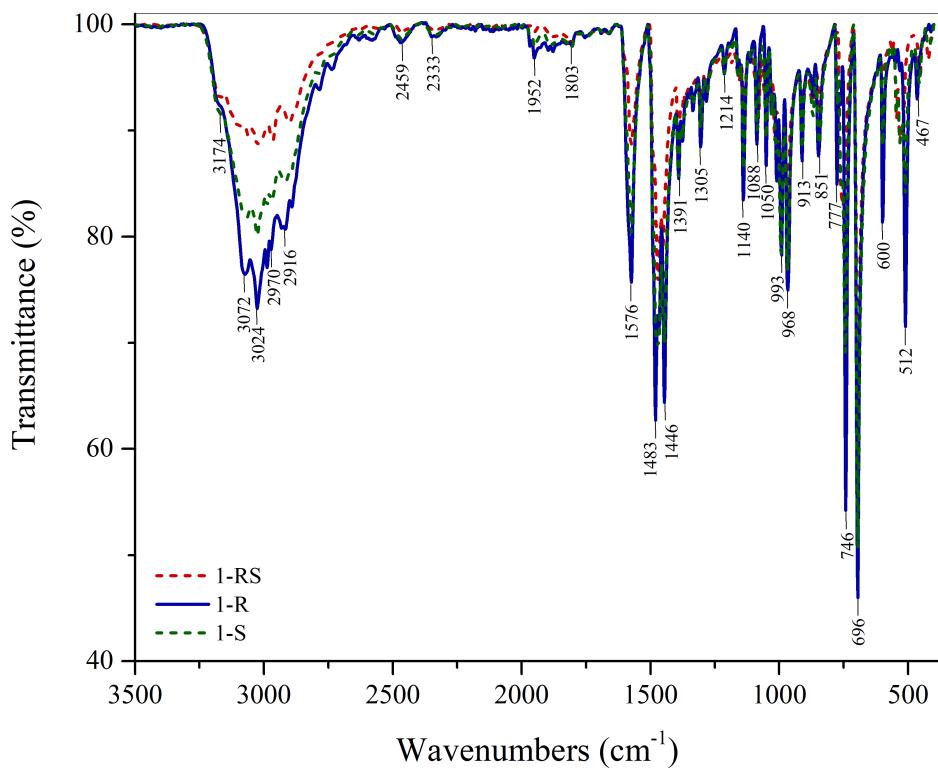
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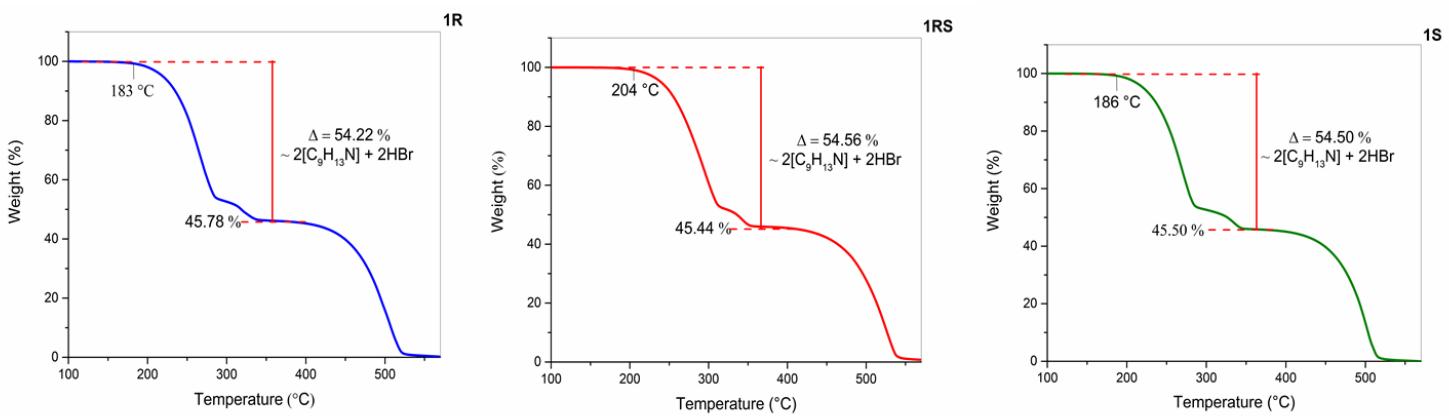
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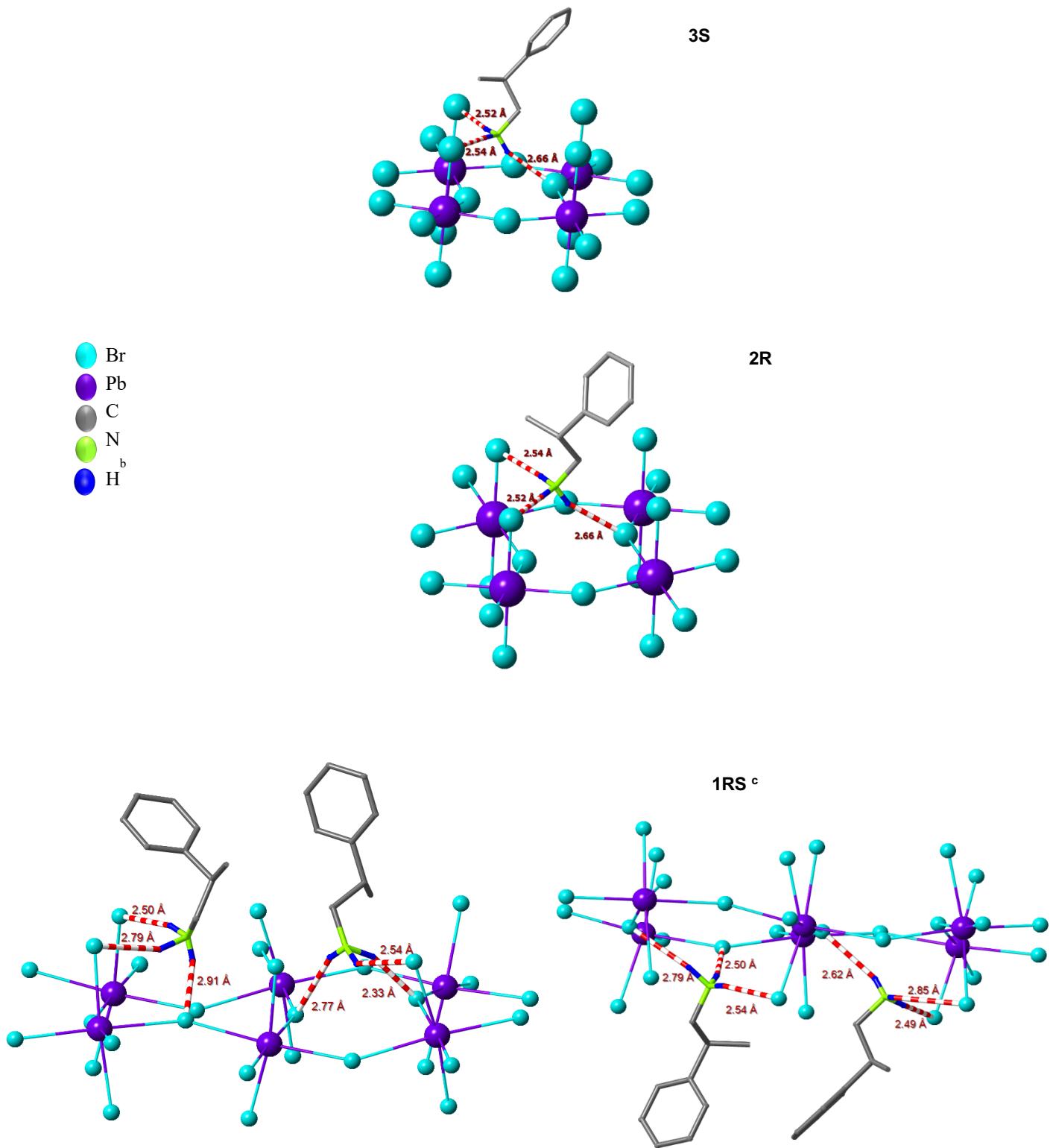
## 1. Figures and Tables



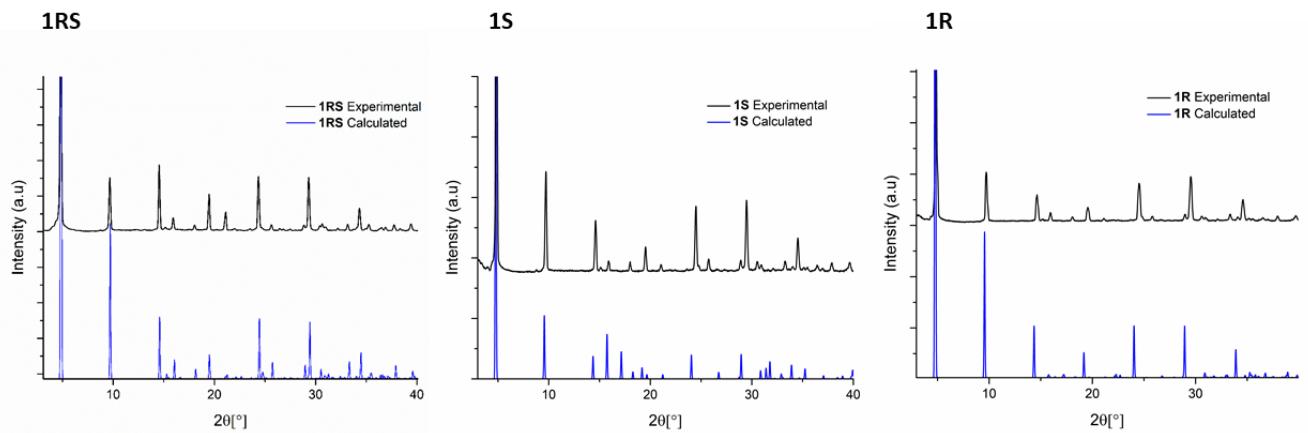
**Figure S1.** FTIR of **1RS**, **1R** and **1S**



**Figure S2.** TGA of **1R**, **1RS** and **1S**



**Figure S3.** Hydrogen bonds (N–H…Br) of **1S**, **1R** and **1RS**. <sup>b</sup> C–H bonds are omitted for clarity. <sup>c</sup> Disorder was omitted for clarity.



**Figure S4.** Experimental and calculated powder X-ray diffraction patterns of **1RS**, **1S** and **1R**.

**Table S1.** Reported Room-Temperature Photoluminescence Quantum Efficiencies (PLQE) and CIE Chromaticity Coordinates for White-Light-Emitting Perovskites

Perovskite	PLQE	CIE	Ref
(EDBE) $\text{PbBr}_4$	9	(0.39, 0.42)	<sup>1</sup>
(EDBE) $\text{PbCl}_4$	2	(0.33, 0.39)	<sup>1</sup>
(CyBMA) $\text{PbBr}_4$	1.5	(0.23, 0.29)	<sup>2</sup>
(N-MEDA) $\text{PbBr}_4$	0.5	(0.36, 0.41)	<sup>3</sup>
(N-MEDA) $\text{PbCl}_{1.2} \text{ Br}_{2.8}$	1.5	--	<sup>3</sup>
(PEA) $_2\text{PbCl}_4$	<1	(0.37, 0.42)	<sup>4</sup>

## 2. X-Ray diffraction data

**Table S2.** Crystal data and structure refinement details for **1R**

Formula	C <sub>18</sub> H <sub>28</sub> Br <sub>4</sub> N <sub>2</sub> Pb
Moiety formula	Br <sub>4</sub> Pb, 2(C <sub>9</sub> H <sub>14</sub> N)
Fw	799.25
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2
Temp, K	100(2)
$\lambda$ , Å	1.54178
<i>a</i> , Å	5.6828(2)
<i>b</i> , Å	36.9869(16)
<i>c</i> , Å	5.6490(3)
$\alpha$ , deg	90
$\beta$ , deg	90
$\gamma$ , deg	90
<i>V</i> , Å <sup>3</sup>	1187.36(9)
Z	2
$\rho$ , g·cm <sup>-3</sup>	2.236
$\mu$ , mm <sup>-1</sup>	21.726
<i>F</i> (000)	744
Crystal size, mm <sup>3</sup>	0.175 x 0.122 x 0.015
Θ range for data collection, deg	1.194 to 72.799
index ranges	$-6 \leq h \leq 7$ $-44 \leq k \leq 45$ $-6 \leq l \leq 6$
No. of reflns collected	17048
No. of indep. reflns ( $R_{\text{int}}$ )	2298 (0.0279)
No. of data / restraints / parameters	2298 / 0 / 127
GoF on $F^2$	1.229
$R_1$ , <sup>a</sup> $wR_2$ , <sup>b</sup> ( $I > 2\sigma(I)$ )	0.0445, 0.1312
Abs. struct. par.	-0.022(8)
Largest diff. peak / hole, e·Å <sup>-3</sup>	2.962 / -2.992

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

**Table S3.** Crystal data and structure refinement details for **1S**

Formula	C <sub>18</sub> H <sub>28</sub> Br <sub>4</sub> N <sub>2</sub> Pb
Moiety formula	Br <sub>4</sub> Pb, 2(C <sub>9</sub> H <sub>14</sub> N)
Fw	799.25
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2
Temp, K	100(2)
$\lambda$ , Å	0.71073
<i>a</i> , Å	5.6922(1)
<i>b</i> , Å	36.9751(7)
<i>c</i> , Å	5.6533(1)
$\alpha$ , deg	90
$\beta$ , deg	90
$\gamma$ , deg	90
<i>V</i> , Å <sup>3</sup>	1189.85(4)
<i>Z</i>	2
$\rho$ , g·cm <sup>-3</sup>	2.231
$\mu$ , mm <sup>-1</sup>	13.811
<i>F</i> (000)	744
Crystal size, mm <sup>3</sup>	0.150 x 0.120 x 0.025
$\theta$ range for data collection, deg	2.203 to 26.369
index ranges	$-7 \leq h \leq 7$ $-46 \leq k \leq 46$ $-7 \leq l \leq 7$
No. of reflns collected	17450
No. of indep. reflns ( <i>R</i> <sub>int</sub> )	2405 (0.0357)
No. of data / restraints / parameters	2405 / 0 / 127
GoF on <i>F</i> <sup>2</sup>	1.038
<i>R</i> <sub>1</sub> , <sup>a</sup> <i>wR</i> <sub>2</sub> , <sup>b</sup> ( <i>I</i> > 2 $\sigma$ ( <i>I</i> ))	0.0146, 0.0300
Abs. struct. par.	0.004(5)
Largest diff. peak / hole, e·Å <sup>-3</sup>	0.823 / -0.817

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

**Table S4.** Crystal data and structure refinement details for **1RS**

Formula	C <sub>18</sub> H <sub>28</sub> Br <sub>4</sub> N <sub>2</sub> Pb
Moiety formula	Br <sub>4</sub> Pb, 2(C <sub>9</sub> H <sub>14</sub> N)
Fw	799.25
Crystal system	orthorhombic
Space group	Pbca
Temp, K	100(2)
$\lambda$ , Å	0.71073
<i>a</i> , Å	33.3990(5)
<i>b</i> , Å	8.0291(1)
<i>c</i> , Å	36.3814(5)
$\alpha$ , deg	90
$\beta$ , deg	90
$\gamma$ , deg	90
<i>V</i> , Å <sup>3</sup>	9756.2(2)
<i>Z</i>	16
$\rho$ , g·cm <sup>-3</sup>	2.177
$\mu$ , mm <sup>-1</sup>	13.475
<i>F</i> (000)	5952
Crystal size, mm <sup>3</sup>	0.4230 x 0.1422 x 0.1271
$\theta$ range for data collection, deg	2.668 to 29.195
index ranges	$-45 \leq h \leq 30$ $-8 \leq k \leq 10$ $-49 \leq l \leq 44$
No. of reflns collected	29461
No. of indep. reflns ( <i>R</i> <sub>int</sub> )	11324 (0.0374)
No. of data / restraints / parameters	11324 / 4356/ 813
GoF on <i>F</i> <sup>2</sup>	1.142
<i>R</i> <sub>1</sub> , <sup>a</sup> <i>wR</i> <sub>2</sub> , <sup>b</sup> ( <i>I</i> > 2 $\sigma$ ( <i>I</i> ))	0.0378, 0.0729
Largest diff. peak / hole, e·Å <sup>-3</sup>	2.210 / -1.861

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

**Table S5.** Pb–Br bond lengths bonds for **1R****1R** Pb–Br lengths/ Å (mal)

Pb1–Br1	2.9803(18)
Pb1–Br1#1	2.9804(18)
Pb1–Br2	2.992(4)
Pb1–Br2#2	2.980(4)
Pb1–Br2#3	2.980(4)
Pb1–Br2#1	2.992(4)
Pb1–Br3	2.9745(14)
Pb1–Br3#4	2.9745(14)
Pb1–Br3A	2.9816(16)
Pb1–Br3A#4	2.9816(16)

#1 –x+1, –y+1, z; #2 –x+1, –y+1, z–1; #3 x, y, z–1; #4 x–1, y, z

**Table S6.** Pb–Br bond lengths bonds for **1S****1 S** Pb–Br lengths/ Å

Pb1–Br1	2.9808(4)
Pb1–Br1#1	2.9809(4)
Pb1–Br2	2.9923(8)
Pb1–Br2#1	2.9922(8)
Pb1–Br2#2	2.9859(8)
Pb1–Br2#3	2.9859(8)
Pb1–Br3	2.9760(3)
Pb1–Br3#4	2.9760(3)
Pb1–Br3#5	2.9865(3)
Pb1–Br3'	2.9865(3)

#1 –x+2, –y+1, z; #2 –x+2, –y+1, z+1; #3 x, y, z+1; #4 x+1, y, z; #5 x–1, y, z

**Table S7.** Pb–Br bond lengths bonds for **1RS****1RS** Pb–Br lengths/ Å

Pb1—Br1	2.9802(5)
Pb1—Br2	2.9848(5)
Pb1—Br3	2.9307(6)
Pb1—Br4	3.0105(5)
Pb1—Br4#1	3.0266(5)
Pb1—Br5	3.0483(5)
Pb2—Br1	3.0482(5)
Pb2—Br2#2	3.0929(6)
Pb2—Br6	3.0234(6)
Pb2—Br7	2.9771(5)
Pb2—Br7#3	2.9843(5)
Pb2—Br8	2.9239(5)

#1 -x+1, y+1/2, -z+3/2; #2 x, y+1, z; #3 -x+1/2, y+1/2, z

**Table S8.** Geometrical parameters of hydrogen bonds for **1R**

<b>1R</b>					
D—H···A	Symmetry code	d <sub>D—H</sub> /Å	d <sub>H···A</sub> /Å	d <sub>D···A</sub> /Å	< <sub>DHA</sub> /°
N1—H1A···Br1	x, y, z-1	0.91	2.52	3.426(19)	171.9
N1—H1B···Br2	x-1, y, z-1	0.91	2.66	3.516(17)	157.0
N1—H1B···Br2	-x+1, -y+1, z-1	0.91	2.97	3.417(16)	112.0
N1—H1B···Br3A	x-1, y, z-1	0.91	2.77	3.417(18)	129.2
N1—H1C···Br1		0.91	2.54	3.449(19)	175.7

**Table S9.** Geometrical parameters of hydrogen bonds for **1S**

<b>1S</b>					
D—H···A	Symmetry code	d <sub>D—H</sub> /Å	d <sub>H···A</sub> /Å	d <sub>D···A</sub> /Å	< <sub>DHA</sub> /°
N1—H1A···Br1	x-1, y, z-1	0.91	2.54	3.454(4)	176.4
N1—H1B···Br2		0.91	2.67	3.520(4)	156.2
N1—H1B···Br2	-x+1, -y+1, z	0.91	2.96	3.406(3)	112.2
N1—H1B···Br3	x, y, z-1	0.91	2.74	3.435(3)	134.0
N1—H1B···Br3'	x-1, y, z	0.91	2.80	3.415(4)	126.3
N1—H1C···Br1	x-1, y, z	0.91	2.52	3.423(4)	172.4

**Table S10.** Geometrical parameters of hydrogen bonds for **1RS**

1RS					
D–H···A	Symmetry code	d <sub>D–H</sub> /Å	d <sub>H···A</sub> /Å	d <sub>D···A</sub> /Å	∠ <sub>DHA</sub> /°
N1–H1A···Br8	x, y–1, z	0.91	2.70	3.53(4)	151.6
N1–H1B···Br1		0.91	2.56	3.39(4)	151.8
N1–H1C···Br8	–x+1/2, y–1/2, z	0.91	2.49	3.36(6)	161.2
N1A–H1D···Br8	x, y–1, z	0.91	2.85	3.51(7)	130.8
N1A–H1E···Br1		0.91	2.62	3.47(6)	155.0
N1A–H1F···Br8	–x+1/2, y–1/2, z	0.91	2.49	3.35(9)	157.8
N2–H2B···Br3		0.91	2.48	3.28(3)	146.6
N2–H2C···Br4	–x+1, y+1/2, –z+3/2	0.91	2.96	3.503(16)	119.9
N2–H2C···Br5	–x+1, y+1/2, –z+3/2	0.91	2.68	3.46(4)	144.4
N2–H2D···Br2	x, y+1, z	0.91	2.59	3.47(4)	162.0
N2A–H2E···Br3		0.91	2.54	3.44(4)	168.6
N2A–H2F···Br4	x, y+1, z	0.91	2.80	3.57(4)	143.6
N2A–H2F···Br4	–x+1, y+1/2, –z+3/2	0.91	3.04	3.468(19)	110.8
N2A–H2F···Br5	–x+1, y+1/2, –z+3/2	0.91	2.91	3.45(4)	119.4
N2A–H2G···Br2	x, y+1, z	0.91	2.50	3.37(4)	158.9
N3–H3B···Br6		0.91	2.40	3.303(10)	170.7
N3–H3C···Br5	x, y+1, z	0.91	2.49	3.316(15)	151.2
N3–H3D···Br4	–x+1, y+1/2, –z+3/2	0.91	2.67	3.464(14)	146.2
N3A–H3E···Br3	–x+1, y+1/2, –z+3/2	0.91	2.79	3.65(3)	158.0
N3A–H3G···Br5	x, y+1, z	0.91	2.50	3.30(4)	147.5
N4–H4B···Br5		0.91	2.42	3.266(12)	154.9
N4–H4C···Br6	x, y–1, z	0.91	2.49	3.347(11)	156.5
N4–H4D···Br1		0.91	2.91	3.497(10)	123.4
N4–H4D···Br7	–x+1/2, y–1/2, z	0.91	2.85	3.445(10)	124.2
N4A–H4E···Br6	x, y–1, z	0.91	2.54	3.19(6)	128.9
N4A–H4F···Br7	–x+1/2, y–1/2, z	0.91	2.33	3.16(5)	152.4
N4A–H4G···Br1		0.91	2.77	3.52(5)	141.0

**Table S11.** Geometrical parameters of hydrogen bonds for  $(\text{PEA})_2\text{PbBr}_4$ <sup>5</sup>

$(\text{PEA})_2\text{PbBr}_4$ <sup>5</sup>				
D—H···A	d <sub>D—H</sub> /Å	d <sub>H···A</sub> /Å	d <sub>D···A</sub> /Å	< <sub>DHA</sub> /°
N1—H1···Br1	0.89	3.18	3.508(5)	104
N1—H3···Br2	0.89	2.54	3.411(5)	165
N2—H13···Br6	0.89	3.17	3.509(5)	105
N2—H14···Br7	0.89	2.54	3.416(5)	167
N3—H26···Br7	0.89	2.71	3.448(6)	142
N3—H27···Br2	0.89	2.62	3.486(6)	164
N4—H37···Br4	0.89	2.68	3.465(5)	148
N4—H39···Br2	0.89	2.73	3.462(6)	140

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