Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting information

Homochiral One-Dimensional ABX_3 Lead Halide Perovskites with High-T_c Quadratic Nonlinear Optical and Dielectric Switchings†

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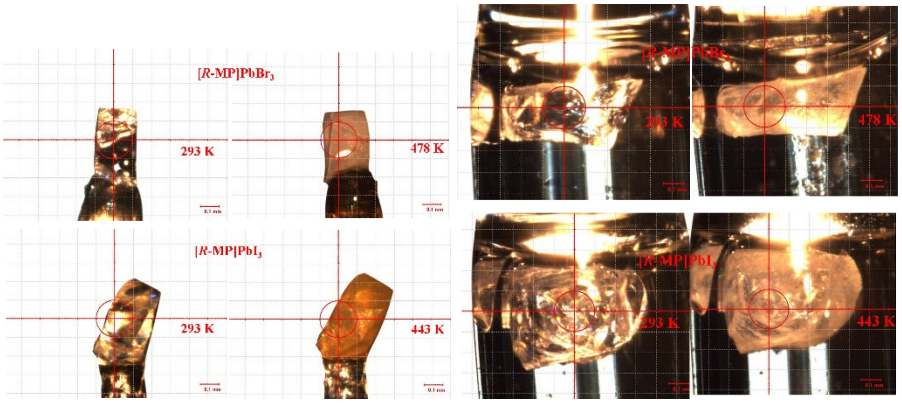

Fig. S1 The change of crystal morphology at different measured temperatures under the flow of warm nitrogen (left) and in a sealed melting point tube (right).

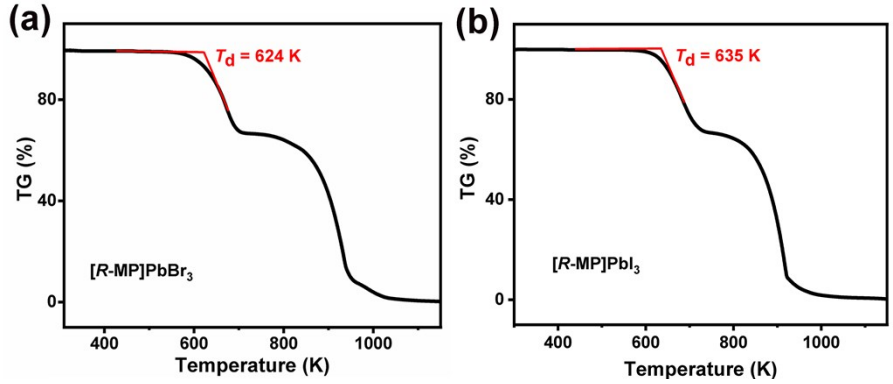

Fig. S2 Thermogravimetric analysis (TGA) curves of [*R*-MP]$PbBr_3$ (a) and [*R*-MP]PbI_3 (b).

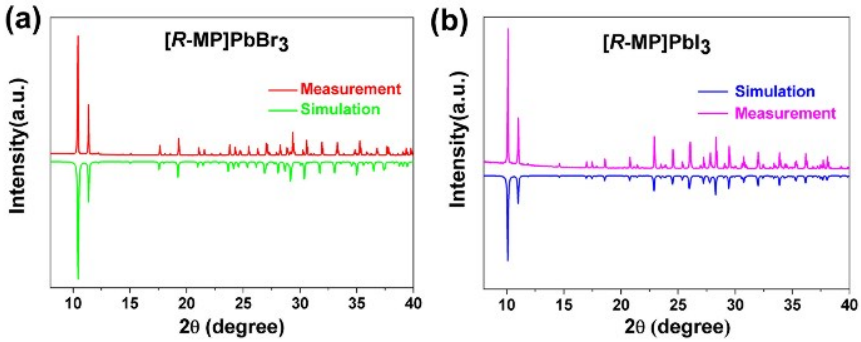

Fig. S3 The measured and simulated PXRD patterns for [*R*-MP]$PbBr_3$ (a) and [*R*-MP]PbI_3 (b) at 293 K.

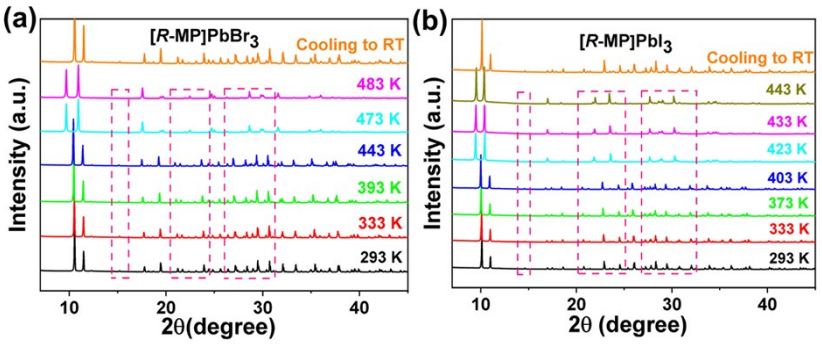

Fig. S4 Variable-temperature PXRD patterns for [*R*-MP]$PbBr_3$ (a) and [*R*-MP]PbI_3 (b).

Table S1. Crystal data and structure refinements for [*R*-MP]$PbBr_3$ and [*R*-MP]PbI_3 at 293 K.

Formula	$[C_6H_{14}N]PbBr_3$	$[C_6H_{14}N]PbI_3$
Temperature	293 K	293 K
Weight	547.10	688.08
Crystal system	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
a/Å	8.1775(3)	8.4004(4)
b/Å	10.0778(5)	10.4483(5)
c/Å	15.5422(6)	16.0931(7)
α/deg	90	90
β/deg	90	90
γ/deg	90	90
Volume/Å^3	1280.85(9)	1412.51(11)
D_c/g cm^{-3}	2.837	3.236
Z	4	4
*R*1 [$I>2\sigma(I)$]	0.0401	0.0432
*wR*2 [$I>2\sigma(I)$]	0.0789	0.1080
GOF	1.003	1.005

Table S2. Selected Pb−Br bond lengths [Å] and Br−Pb−Br bond angles [°] for [*R*-MP]$PbBr_3$ at 293 K.

Bond lengths [Å]		Bond angles [°]			
Pb1−Br1	2.9042(15)	Br1^{i}−Pb1−Br3	84.888(40)	Br1^{i}−Pb1−Br3^{ii}	106.313(36)
Pb1−Br2	2.9443(14)	Br1−Pb1−Br2	87.02(4)	Br1^{i}−Pb1−Br2^{ii}	75.150(38)
Pb1−Br3	2.8465(15)	Br1−Pb1−Br2^{ii}	98.552(41)	Br2−Pb1−Br3	90.34(4)
Pb1−Br1^{i}	3.2692(15)	B1r−Pb1−Br3	87.62(4)	Br2−Pb1−Br3^{ii}	79.984(38)
Pb1−Br2^{i}	3.3335(15)	Br1−Pb1−Br3^{ii}	81.916(39)	Br2^{ii}−Pb1−Br3	82.276(38)
Pb1−Br3^{ii}	3.3857(14)	Br1^{i}−Pb1−Br2	98.362(41)	Br2^{ii}−Pb1−Br3^{ii}	108.295(36)

Symmetry code(s): (i) -1/2+x, 3/2-y, 1-z; (ii) 1/2+x, 3/2 -y, 1-z.

Table S3. Selected Pb−I bond lengths [Å] and I−Pb−I bond angles [°] for [*R*-MP]PbI_3 at 293 K.

Bond lengths [Å]		Bond angles [°]			
Pb1−I1	3.16(15)	I1^{i}−Pb1−I3	78.692(37)	I1^{i}−Pb1−I3^{ii}	94.825(40)
Pb1−I2	3.0404(15)	I1−Pb1−I2	92.14(4)	I1^{i}−Pb1−I2^{ii}	102.567(37)
Pb1−I3	3.4053(15)	I1−Pb1−I2^{ii}	81.131(37)	I2−Pb1−I3	85.96(3)
Pb1−I1^{i}	3.4306(16)	I1−Pb1−I3	98.42(4)	I2−Pb1−I3^{ii}	88.49(4)
Pb1−I2^{ii}	3.5291(15)	I1−Pb1−I3^{ii}	87.77(4)	I2^{ii}−Pb1−I3	103.044(36)
Pb1−I3^{ii}	3.0888(14)	I1^{i}−Pb1−I2	84.510(38)	I2^{ii}−Pb1−I3^{ii}	83.112(37)

Symmetry code(s): (i) 1/2+x, -1/2-y, -z; (ii) -1/2+x, -1/2 -y, -z.