Dual switching of dielectric and SHG triggered by thermal driven helical axis transformation with fluorescence characteristics

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Experimental measurement methods

X-ray diffraction studies single-crystal diffraction (SC-XRD)

To deeply study the mechanism of phase transition, single crystal structure was the most significant characterization method. In order to get variable-temperature single crystal X-ray diffraction date, we utilized a Rigaku single-crystal X-ray diffractometer using Mo-Kα radiation (λ =0.71073 Å) at 245K, 330K for compound 1 and 263K, 293K, 323K for compound 2. The direct method was employed to solve the crystallographic structure at different temperatures, and we made use of the SHELXTL-2014 program package to correct it by the full matrix least squares method.

Variable-temperature X-ray powder diffraction (VT-PXRD)

Variable-temperature powder X-ray diffraction measurements was characterized from 230 to 330K using a Rigaku D/MAX 2000 PC X-ray diffractometer. The test conditions range from 5 to 50 with a step of 0.02°. The test temperature range for compound 1 is 245-330K, while the test temperature range is 243-333K for compound 2, and corresponding PXRD patterns were obtained.

Differential scanning calorimetry (DSC)

To prove the reversible phase transitions of (N, N-dimethyl-pyrrolidinium)$PbCl_3$ (compound 1), and (N, N-dimethyl-pyrrolidinium)$PbBr_3$ (compound 2), DSC measurement was performed by using a Perkin-Elmer DSC instrument in a nitrogen atmosphere. During a heating and cooling cycle, the powder samples were studied in the temperature range of 240 K to 340 K with a rate of 15 K min^{-1}, when added to alumina crucible (sample 1:11.5mg, sample 2: 10.1mg).

The complex dielectric permittivity

For the dielectric measurements, the crystal was ground into powder and pressed into a sheet of about 0.5 mm in thickness. And the sheet was fixed on the electrode with silver glue, covering an area of about 10 mm^{-2}. The complex dielectric constant ε (ε = ε'- iε'') was obtained by the TH2828A instrument and should be lower than the melting point of the compound.

Infrared (IR) measurement

The IR measurement was carried out by using a Shimadzu model IR-60 spectrometer at room temperature. Prior to the experiments, the sample was mixed with KBr and ground into a powder, and then it was pressed into a thin and transparent sheet.

SHG measurements.

The compounds were prepared into powders with different particle sizes for SHG response testing. Temperature-varying SHG experiments were performed by using a low-divergence basic laser beam, which pulsed in Nd: YAG. The wavelength is 1064 nm, the peak power is 1.6 MW, the repetition rate is 10 Hz, and the pulse duration is 5 ns.

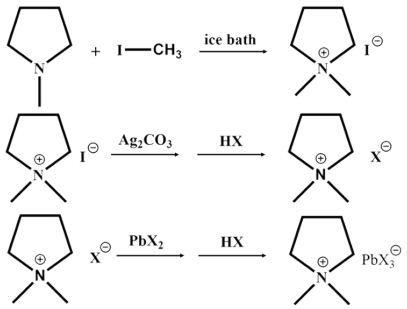

Fig. S1 Specific reaction equation.

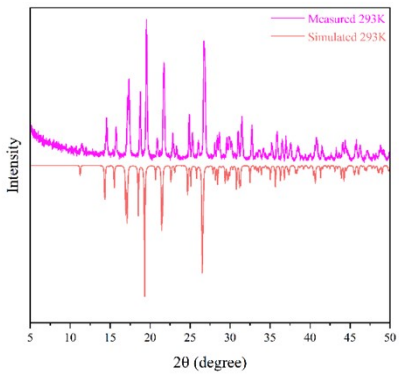

Fig. S2 Measured and simulated powder X-ray diffraction patterns of N, N-Dimethyl pyrrolidinium iodide at 293 K.

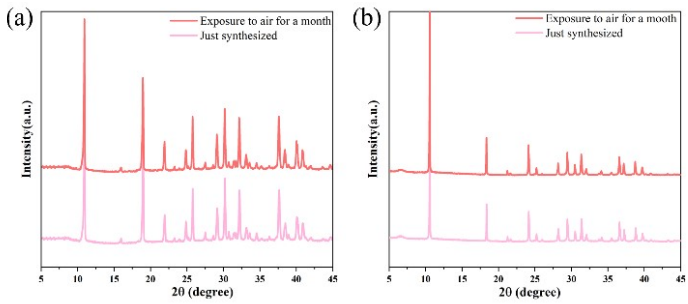

Fig. S3 Comparison of powder diffraction patterns of compounds 1 (a) and 2 (b) before and after exposure to air.

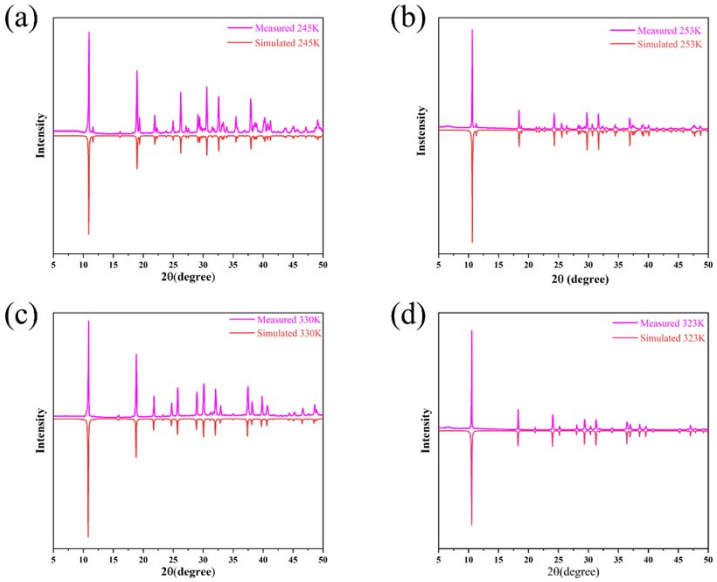

Fig. S4 Measured and simulated powder X-ray diffraction patterns of compound 1 at 245 K (a) and 330 K (c); compound 2 at 253 K (b) and 323K (d).

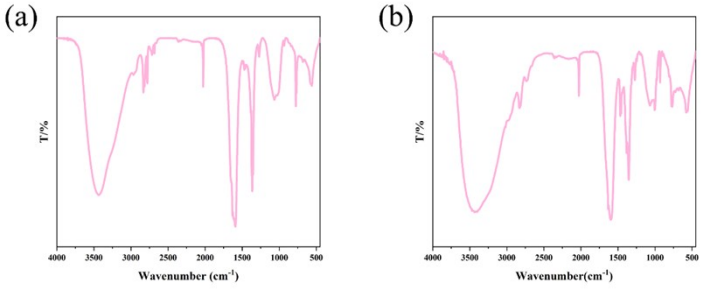

Fig. S5 Infrared spectrum of compound 1 (a) and compound 2.

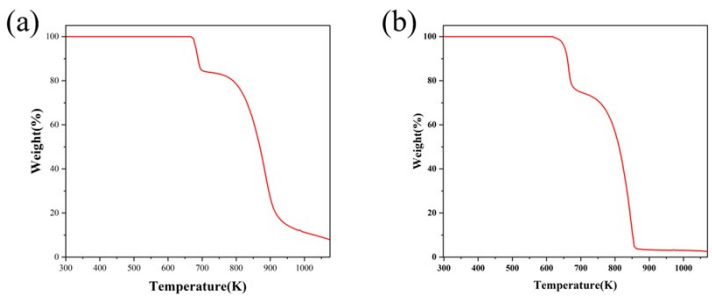

Fig. S6 TGA of the compound of compound 1 (a) and compound 2 (b).

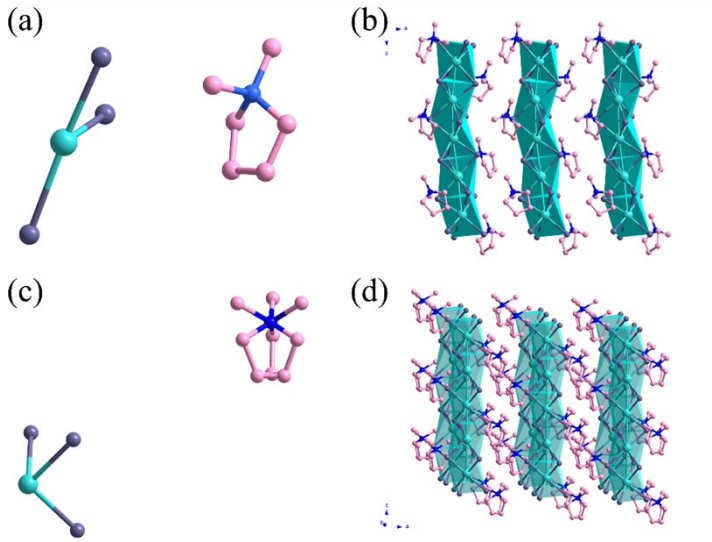

Fig. S7 Asymmetric unit diagram of compound 1 in the LTP (a) and the HTP (c). The packing structure of compound 1 in the LTP (b) and the HTP (d).

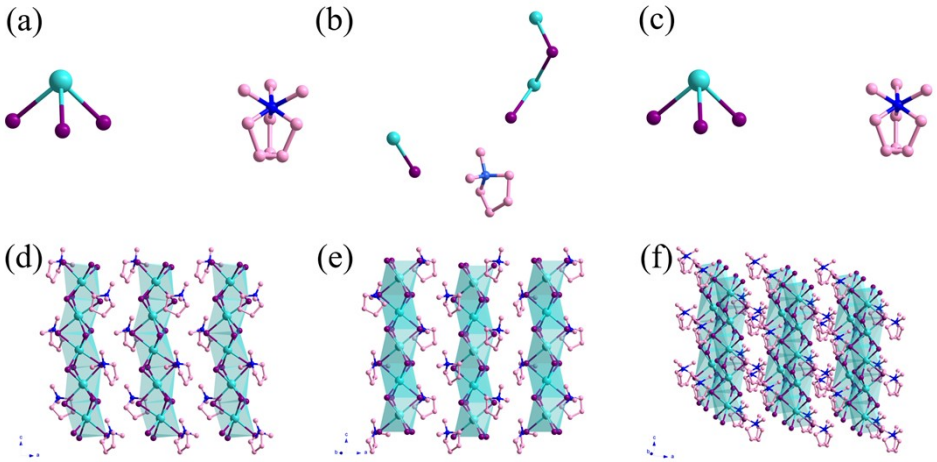

Fig. S8 Asymmetric unit diagram of compound 2 in the LTP (a), RTP (b) and HTP (c). The packing structure of compound 2 in the LTP (d), RTP (e) and HTP (f).

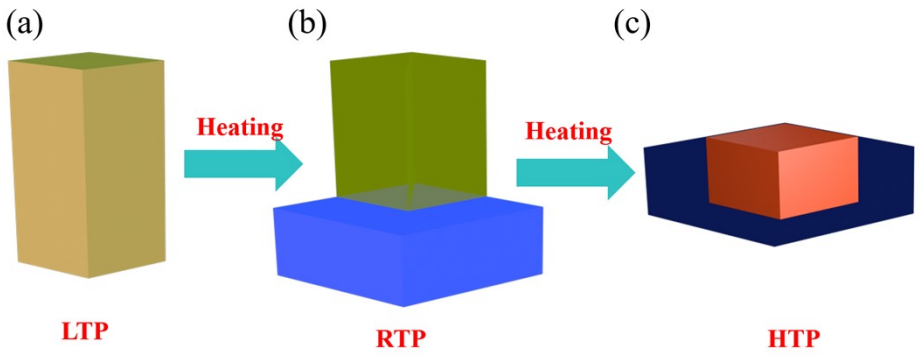

Fig. S9 Schematic diagram of the change in crystal cell volume of compound compound 2.

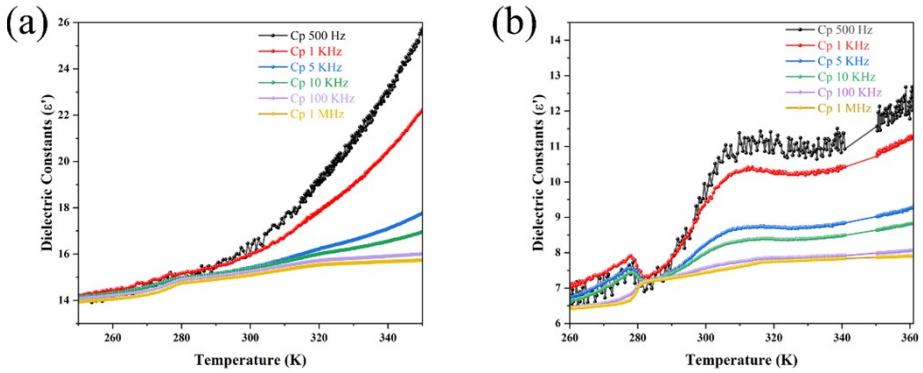

Fig. S10 Dielectric constant of compound 1 (a) and compound 2 (b) at different frequencies.

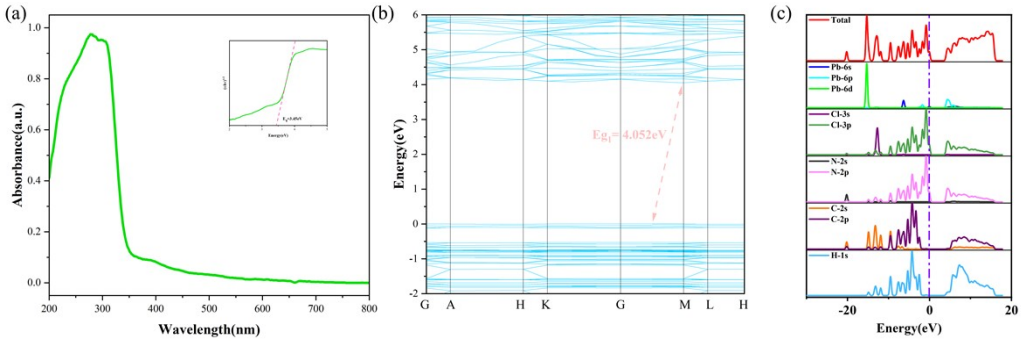

Fig. S11 UV-vis absorption spectra of compound 1 and the inset show the Tauc plots (a). The calculated band structures and PDOS of compound 1 (b and c).

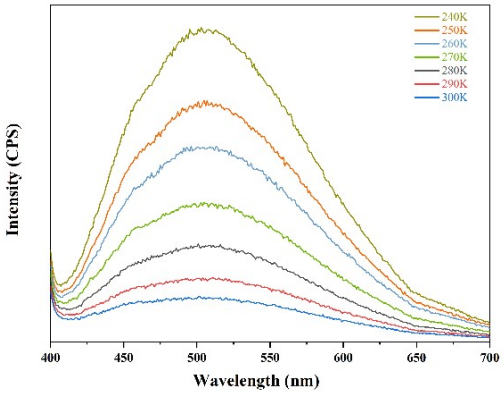

Fig. S12 Temperature-dependent PL spectra of compound 2.

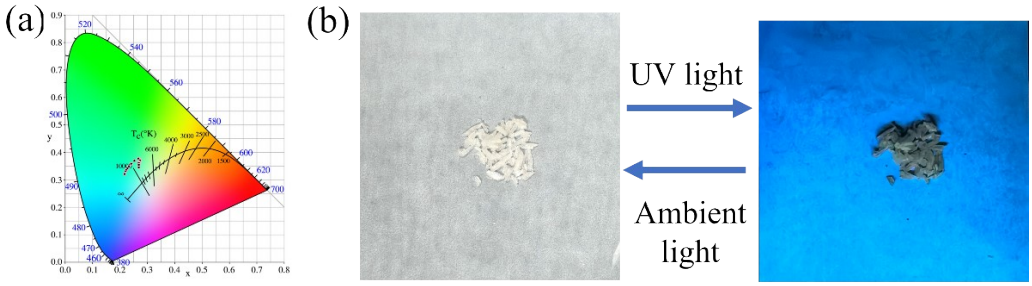

Fig. S13 CIE chromaticity coordinates of compound 2 (a). Color changes under UV light irradiation at room temperature (b).

Table. S1 The chemical elemental analysis test results are shown in the table.

	Calculated results (%)	Experimental results (%)
Compound 1	C:17.41 N:3.38 H:3.42	C:17.38 N:3.43 H:3.42
Compound 2	C:13.17 N:2.56 H:2.58	C:13.21 N:2.61 H:2.56

Table. S2 Crystal data and structure refinements for (N, N-dimethyl pyrrolidinium)$PbCl_3$ at 245 K and 330 K.

Compound	(N, N-dimethyl pyrrolidinium)$PbCl_3$	
Temperature	245 K	330 K
Formula	$[C_6H_{14}N]PbCl_3$	$[C_6N]PbCl_3$
Formula weight	413.72	399.61
Crystal system	hexagonal	hexagonal
Space group	$P6_1$	$P6_3mc$
a, b, c (Å)	9.3571(10)	9.4432(4)
	9.3571(10)	9.4432(4)

	22.408(4)	7.6506(5)
α, β, γ (°)	90	90
	90	90
	120	120
Volume /Å3	1699.1(5)	590.83(6)
Z	6	2
Density/g cm^{-3}	2.462	2.246
R_1	0.0262	0.0299
wR_2	0.0568	0.0916
GOF	1.038	1.060

Table. S3 Crystal data and structure refinements for (N, N-dimethyl pyrrolidinium)$PbBr_3$ at 253 K, 293 K and 323 K.

Compound	(N, N-dimethyl pyrrolidinium)$PbBr_3$		
Temperature	253 K	293 K	323 K
Formula	$[C_6H_{14}N]PbBr_3$	$[C_{18}H_{24}N_3]Pb_3Br_9$	$[C_6N]PbBr_3$
Formula weight	547.10	1641.30	532.99
Crystal system	hexagonal	hexagonal	hexagonal
Space group	$P6_1$	$P6_3$	$P6_3mc$
a, b, c (Å)	9.6156(3)	16.7130(7)	9.7180(6)
	9.6156(3)	16.7130(7)	9.7180(6)
	22.9958(11)	7.7768(10)	7.7965(12)
α, β, γ (°)	90	90	90
	90	90	90
	120	120	120
Volume /Å3	1841.33(14)	1881.2(3)	637.65(13)
Z	6	2	2
Density/g cm^{-3}	2.960	2.898	2.776
R_1	0.0408	0.0547	0.0546
wR_2	0.0830	0.1319	0.1363
GOF	1.017	1.001	1.123

Table S4. Bond Lengths and Bond Angles for (N, N-dimethyl pyrrolidinium)$PbCl_3$ at 245 K and 330 K.

Bond lengths [Å] and angles [°]			
245 K			
Pb1—Cl1	2.862 (3)	C2—H2B	0.9800
Pb1—$Cl1^i$	2.918 (3)	C2—C3	1.515 (18)
Pb1—Cl2	2.890 (4)	C3—H3A	0.9800
Pb1—$Cl2^i$	2.873 (4)	C3—H3B	0.9800

Pb1—Cl3^{ii}	2.930 (3)	C3—C4	1.514 (19)
Pb1—Cl3	2.940 (3)	C4—H4A	0.9800
N1—C1	1.492 (15)	C4—H4B	0.9800
N1—C4	1.481 (15)	C5—H5A	0.9700
N1—C5	1.503 (14)	C5—H5B	0.9700
N1—C6	1.502 (18)	C5—H5C	0.9700
C1—H1A	0.9800	C6—H6A	0.9700
C1—H1B	0.9800	C6—H6B	0.9700
C1—C2	1.501 (18)	C6—H6C	0.9700
C2—H2A	0.9800		

Cl1—Pb1—Cl1^{i}	94.19 (7)	C1—C2—H2A	110.7
Cl1—Pb1—Cl2	84.63 (9)	C1—C2—H2B	110.7
Cl1—Pb1—Cl2^{i}	93.67 (8)	C1—C2—C3	105.2 (11)
Cl1^{i}—Pb1—Cl3^{ii}	99.90 (11)	H2A—C2—H2B	108.8
Cl1—Pb1—Cl3^{ii}	81.91 (10)	C3—C2—H2A	110.7
Cl1—Pb1—Cl3	173.34 (10)	C3—C2—H2B	110.7
Cl1^{i}—Pb1—Cl3	80.82 (9)	C2—C3—H3A	110.6
Cl2—Pb1—Cl1^{i}	178.14 (8)	C2—C3—H3B	110.6
Cl2^{i}—Pb1—Cl1^{i}	83.91 (10)	H3A—C3—H3B	108.7
Cl2^{i}—Pb1—Cl2	94.73 (7)	C4—C3—C2	105.8 (12)
Cl2^{i}—Pb1—Cl3	81.47 (11)	C4—C3—H3A	110.6
Cl2^{i}—Pb1—Cl3^{ii}	174.33 (11)	C4—C3—H3B	110.6
Cl2—Pb1—Cl3^{ii}	81.36 (10)	N1—C4—C3	104.0 (10)
Cl2—Pb1—Cl3	100.25 (11)	N1—C4—H4A	110.9
Cl3^{ii}—Pb1—Cl3	103.20 (5)	N1—C4—H4B	110.9
Pb1—Cl1—Pb1^{ii}	81.38 (9)	C3—C4—H4A	110.9
Pb1^{ii}—Cl2—Pb1	81.68 (9)	C3—C4—H4B	110.9
Pb1^{i}—Cl3—Pb1	79.88 (6)	H4A—C4—H4B	109.0
C1—N1—C5	109.8 (9)	N1—C5—H5A	109.5
C1—N1—C6	113.2 (11)	N1—C5—H5B	109.5

C4—N1—C1	102.6 (10)	N1—C5—H5C	109.5
C4—N1—C5	110.5 (10)	H5A—C5—H5B	109.5
C4—N1—C6	112.0 (10)	H5A—C5—H5C	109.5
C6—N1—C5	108.6 (10)	H5B—C5—H5C	109.5
N1—C1—H1A	110.9	N1—C6—H6A	109.5
N1—C1—H1B	110.9	N1—C6—H6B	109.5
N1—C1—C2	104.5 (10)	N1—C6—H6C	109.5
H1A—C1—H1B	108.9	H6A—C6—H6B	109.5
C2—C1—H1A	110.9	H6A—C6—H6C	109.5
C2—C1—H1B	110.9	H6B—C6—H6C	109.5

Symmetry codes: (i) $x-y+1, x-1, z+1/6$; (ii) $y+1, -x+y+2, z-1/6$.

Bond lengths [Å] and angles [°]			
330 K			
Pb1—Cl1^{i}	2.88 (3)	N1—C2^{vii}	1.406 (13)
Pb1—Cl1	2.93 (3)	N1—C3	1.707 (14)
Pb1—Cl1^{ii}	2.88 (3)	N1—C3^{vi}	1.707 (14)
Pb1—Cl1^{iii}	2.93 (3)	N1—C3^{vii}	1.707 (14)
Pb1—Cl1^{iv}	2.93 (3)	C1—C1^{vi}	1.05 (9)
Pb1—Cl1^{v}	2.88 (3)	C1—C1^{vii}	1.05 (9)
N1—C2^{vi}	1.406 (14)	C1—C2	1.610 (14)
N1—C2	1.406 (14)	C2—C3	1.493 (14)
Cl1^{i}—Pb1—Cl1^{v}	82.2 (10)	C2^{vi}—N1—C3	127.6 (2)
Cl1^{v}—Pb1—Cl1	98.60 (7)	C2^{vii}—N1—C3^{vi}	127.6 (2)
Cl1^{i}—Pb1—Cl1^{iv}	179.0 (13)	C2^{vi}—N1—C3^{vi}	56.3 (7)
Cl1—Pb1—Cl1^{iv}	80.6 (10)	C2—N1—C3^{vi}	127.6 (2)
Cl1^{ii}—Pb1—Cl1	179.0 (13)	C2—N1—C3^{vii}	127.6 (2)
Cl1—Pb1—Cl1^{iii}	80.6 (10)	C2^{vi}—N1—C3^{vii}	127.6 (2)
Cl1^{i}—Pb1—Cl1	98.60 (7)	C2^{vii}—N1—C3^{vii}	56.3 (7)
Cl1^{i}—Pb1—Cl1^{ii}	82.2 (10)	C2—N1—C3	56.3 (7)
Cl1^{ii}—Pb1—Cl1^{iii}	98.60 (7)	C2^{vii}—N1—C3	127.6 (2)

Cl1^{v}—Pb1—Cl1^{iii}	179.0 (13)	C3—N1—C3^{vi}	98 (2)
Cl1^{iv}—Pb1—Cl1^{iii}	80.6 (10)	C3^{vi}—N1—C3^{vii}	98 (2)
Cl1^{v}—Pb1—Cl1^{ii}	82.2 (10)	C3—N1—C3^{vii}	98 (2)
Cl1^{ii}—Pb1—Cl1^{iv}	98.60 (7)	C1^{vi}—C1—C1^{vii}	60.001 (2)
Cl1^{v}—Pb1—Cl1^{iv}	98.60 (7)	C1^{vi}—C1—C2	110.3 (13)
Cl1^{i}—Pb1—Cl1^{iii}	98.60 (7)	C1^{vii}—C1—C2	110.3 (13)
Pb1^{viii}—Cl1—Pb1	82.31 (9)	N1—C2—C1	93.4 (11)
C2^{vi}—N1—C2	101.0 (19)	N1—C2—C3	72.1 (9)
C2^{vi}—N1—C2^{vii}	101.0 (19)	C3—C2—C1	165.5 (16)
C2—N1—C2^{vii}	101.0 (19)	C2—C3—N1	51.6 (7)

Symmetry codes: (i) *y*+1, −*x*+*y*+1, *z*+1/2; (ii) −*x*+2, −*y*, *z*+1/2; (iii) −*x*+*y*+2, −*x*+1, *z*; (iv) −*y*+1, *x*−*y*−1,

Table S5. Bond Lengths and Bond Angles for (N, N-dimethyl pyrrolidinium)$PbBr_3$ at 253 K, 293 K and 323 K.

Bond lengths [Å] and angles [°]			
253 K			
Pb1—Br1^{i}	3.0055 (15)	C2—H2B	0.9800
Pb1—Br1	3.0129 (16)	C2—C3	1.55 (2)
Pb1—Br2^{i}	3.0414 (16)	C3—H3A	0.9800
Pb1—Br2	2.9939 (15)	C3—H3B	0.9800
Pb1—Br3	3.0526 (17)	C3—C4	1.51 (2)
Pb1—Br3^{i}	3.0654 (17)	C4—H4A	0.9800
N1—C1	1.506 (19)	C4—H4B	0.9800
N1—C4	1.514 (15)	C5—H5A	0.9700
N1—C5	1.43 (2)	C5—H5B	0.9700
N1—C6	1.509 (18)	C5—H5C	0.9700
C1—H1A	0.9800	C6—H6A	0.9700
C1—H1B	0.9800	C6—H6B	0.9700
C1—C2	1.52 (2)	C6—H6C	0.9700
C2—H2A	0.9800		
Br1^{i}—Pb1—Br1	93.72 (3)	C1—C2—H2A	110.6
Br1—Pb1—Br2^{i}	178.92 (4)	C1—C2—H2B	110.6
Br1^{i}—Pb1—Br2^{i}	85.41 (4)	C1—C2—C3	105.7 (13)

Br1^{i}—Pb1—Br3^{i}	82.77 (5)	H2A—C2—H2B	108.7
Br1—Pb1—Br3	82.86 (5)	C3—C2—H2A	110.6
Br1^{i}—Pb1—Br3	175.00 (5)	C3—C2—H2B	110.6
Br1—Pb1—Br3^{i}	98.55 (4)	C2—C3—H3A	110.8
Br2—Pb1—Br1^{i}	93.19 (4)	C2—C3—H3B	110.8
Br2—Pb1—Br1	86.12 (4)	H3A—C3—H3B	108.9
Br2—Pb1—Br2^{i}	93.30 (3)	C4—C3—C2	104.8 (12)
Br2^{i}—Pb1—Br3^{i}	81.97 (4)	C4—C3—H3A	110.8
Br2—Pb1—Br3	82.96 (5)	C4—C3—H3B	110.8
Br2^{i}—Pb1—Br3	97.98 (4)	N1—C4—H4A	110.5
Br2—Pb1—Br3^{i}	173.99 (5)	N1—C4—H4B	110.5
Br3—Pb1—Br3^{i}	101.31 (3)	C3—C4—N1	106.2 (12)
Pb1^{ii}—Br1—Pb1	79.80 (3)	C3—C4—H4A	110.5
Pb1—Br2—Pb1^{ii}	79.53 (3)	C3—C4—H4B	110.5
Pb1—Br3—Pb1^{ii}	78.25 (3)	H4A—C4—H4B	108.7
C1—N1—C4	101.9 (10)	N1—C5—H5A	109.5
C1—N1—C6	107.7 (11)	N1—C5—H5B	109.5
C5—N1—C1	113.2 (12)	N1—C5—H5C	109.5
C5—N1—C4	115.3 (12)	H5A—C5—H5B	109.5
C5—N1—C6	109.8 (12)	H5A—C5—H5C	109.5
C6—N1—C4	108.5 (10)	H5B—C5—H5C	109.5
N1—C1—H1A	110.6	N1—C6—H6A	109.5
N1—C1—H1B	110.6	N1—C6—H6B	109.5
N1—C1—C2	105.7 (11)	N1—C6—H6C	109.5
H1A—C1—H1B	108.7	H6A—C6—H6B	109.5
C2—C1—H1A	110.6	H6A—C6—H6C	109.5
C2—C1—H1B	110.6	H6B—C6—H6C	109.5

Symmetry codes: (i) $y+1, -x+y+1, z-1/6$; (ii) $x-y, x-1, z+1/6$.

Bond lengths [Å] and angles [°]

293 K			
Pb1—Br1	3.007 (3)	N1—C5	1.458 (11)
Pb1—Br1^{i}	3.047 (3)	N1—C6	1.462 (9)
Pb1—Br1^{ii}	3.047 (3)	C1—H1A	0.9700
Pb1—Br1^{iii}	3.007 (3)	C1—H1B	0.9700
Pb1—Br1^{iv}	3.007 (3)	C1—C2	1.533 (11)
Pb1—Br1^{v}	3.047 (3)	C2—H2A	0.9700
Pb2—Br2	3.031 (5)	C2—H2B	0.9700
Pb2—Br2^{vi}	3.031 (5)	C2—C3	1.528 (10)
Pb2—Br2^{vii}	3.031 (5)	C3—H3A	0.9700
Pb2—Br3^{vii}	3.023 (5)	C3—H3B	0.9700
Pb2—Br3^{vi}	3.023 (4)	C3—C4	1.540 (11)
Pb2—Br3	3.023 (4)	C4—H4A	0.9700
Pb3—Br2^{viii}	3.030 (5)	C4—H4B	0.9700
Pb3—Br2^{ix}	3.030 (5)	C5—H5A	0.9600
Pb3—Br2^{x}	3.030 (5)	C5—H5B	0.9600
Pb3—Br3^{vii}	3.025 (5)	C5—H5C	0.9600
Pb3—Br3^{vi}	3.025 (5)	C6—H6A	0.9600
Pb3—Br3	3.025 (5)	C6—H6B	0.9601
N1—C1	1.460 (10)	C6—H6C	0.9600
N1—C4	1.484 (11)		
Br1—Pb1—Br1^{iii}	83.86 (10)	Br3^{vi}—Pb3—Br3	82.87 (14)
Br1^{iv}—Pb1—Br1^{i}	96.82 (6)	Pb3^{xii}—Br2—Pb2	79.55 (10)
Br1^{iv}—Pb1—Br1^{v}	179.08 (11)	Pb2—Br3—Pb3	80.28 (10)
Br1—Pb1—Br1^{iv}	83.86 (10)	C1—N1—C4	109.1 (12)
Br1—Pb1—Br1^{v}	96.82 (6)	C1—N1—C6	108.3 (11)
Br1^{iii}—Pb1—Br1^{iv}	83.86 (10)	C5—N1—C1	115.8 (16)
Br1^{iii}—Pb1—Br1^{i}	179.08 (11)	C5—N1—C4	114.1 (15)
Br1—Pb1—Br1^{ii}	179.08 (11)	C5—N1—C6	103.0 (15)
Br1^{ii}—Pb1—Br1^{i}	82.50 (10)	C6—N1—C4	105.7 (12)
Br1^{iii}—Pb1—Br1^{ii}	96.82 (6)	N1—C1—H1A	113.9

Br1^{iii}—Pb1—Br1^{v}	96.82 (6)	N1—C1—H1B	113.9
Br1^{iv}—Pb1—Br1^{ii}	96.82 (6)	N1—C1—C2	88.3 (9)
Br1^{ii}—Pb1—Br1^{v}	82.50 (10)	H1A—C1—H1B	111.1
Br1—Pb1—Br1^{i}	96.82 (6)	C2—C1—H1A	113.9
Br1^{i}—Pb1—Br1^{v}	82.50 (10)	C2—C1—H1B	113.9
Pb1—Br1—Pb1^{xi}	79.92 (8)	C1—C2—H2A	109.1
Br2^{vii}—Pb2—Br2^{vi}	83.44 (14)	C1—C2—H2B	109.1
Br2^{vii}—Pb2—Br2	83.44 (14)	H2A—C2—H2B	107.8
Br2^{vi}—Pb2—Br2	83.44 (14)	C3—C2—C1	112.6 (11)
Br3^{vi}—Pb2—Br2^{vi}	96.69 (11)	C3—C2—H2A	109.1
Br3^{vi}—Pb2—Br2	179.63 (14)	C3—C2—H2B	109.1
Br3—Pb2—Br2	96.69 (11)	C2—C3—H3A	111.7
Br3^{vi}—Pb2—Br2^{vii}	96.92 (10)	C2—C3—H3B	111.7
Br3^{vii}—Pb2—Br2	96.92 (10)	C2—C3—C4	100.4 (10)
Br3—Pb2—Br2^{vi}	96.92 (10)	H3A—C3—H3B	109.5
Br3—Pb2—Br2^{vii}	179.63 (14)	C4—C3—H3A	111.7
Br3^{vii}—Pb2—Br2^{vii}	96.69 (11)	C4—C3—H3B	111.7
Br3^{vii}—Pb2—Br2^{vi}	179.63 (14)	N1—C4—C3	93.5 (10)
Br3^{vi}—Pb2—Br3	82.95 (14)	N1—C4—H4A	113.0
Br3^{vii}—Pb2—Br3	82.95 (14)	N1—C4—H4B	113.0
Br3^{vi}—Pb2—Br3^{vii}	82.95 (14)	C3—C4—H4A	113.0
Br2^{ix}—Pb3—Br2^{viii}	83.47 (14)	C3—C4—H4B	113.0
Br2^{viii}—Pb3—Br2^{x}	83.47 (14)	H4A—C4—H4B	110.4
Br2^{ix}—Pb3—Br2^{x}	83.47 (14)	N1—C5—H5A	109.5
Br3^{vi}—Pb3—Br2^{ix}	96.95 (10)	N1—C5—H5B	109.5
Br3^{vii}—Pb3—Br2^{viii}	179.57 (15)	N1—C5—H5C	109.5
Br3^{vi}—Pb3—Br2^{x}	179.57 (14)	H5A—C5—H5B	109.5
Br3^{vii}—Pb3—Br2^{ix}	96.71 (11)	H5A—C5—H5C	109.5
Br3—Pb3—Br2^{viii}	96.95 (10)	H5B—C5—H5C	109.5
Br3—Pb3—Br2^{ix}	179.57 (14)	N1—C6—H6A	109.9
Br3—Pb3—Br2^{x}	96.71 (11)	N1—C6—H6B	108.4

Br3^{vi}—Pb3—Br2^{viii}	96.71 (11)	N1—C6—H6C	110.1
Br3^{vii}—Pb3—Br2^{x}	96.95 (10)	H6A—C6—H6B	109.5
Br3^{vi}—Pb3—Br3^{vii}	82.87 (14)	H6A—C6—H6C	109.5
Br3^{vii}—Pb3—Br3	82.87 (14)	H6B—C6—H6C	109.5

Symmetry codes: (i) *x*−*y*, *x*, *z*+1/2; (ii) −*x*, −*y*, *z*+1/2; (iii) −*x*+*y*, −*x*, *z*; (iv) −*y*, *x*−*y*, *z*; (v) *y*, −*x*+*y*, *z*+1/2;

Bond lengths [Å] and angles [°]			
323 K			
Pb1—Br1^{i}	3.018 (14)	N1—C2	1.402 (14)
Pb1—Br1^{ii}	3.047 (16)	N1—C3	1.700 (14)
Pb1—Br1^{iii}	3.047 (16)	N1—C3^{vii}	1.700 (14)
Pb1—Br1^{iv}	3.018 (14)	N1—C3^{vi}	1.700 (14)
Pb1—Br1	3.018 (14)	C1—C1^{vi}	1.02 (15)
Pb1—Br1^{v}	3.047 (16)	C1—C1^{vii}	1.02 (14)
N1—C2^{vi}	1.402 (14)	C1—C2	1.602 (14)
N1—C2^{vii}	1.402 (14)	C2—C3	1.501 (14)
Br1^{i}—Pb1—Br1^{iv}	83.6 (5)	C2^{vi}—N1—C3	127.8 (2)
Br1^{v}—Pb1—Br1^{iii}	82.6 (5)	C2—N1—C3^{vi}	127.8 (2)
Br1^{v}—Pb1—Br1^{ii}	82.6 (5)	C2^{vi}—N1—C3^{vii}	127.8 (2)
Br1^{i}—Pb1—Br1	83.6 (5)	C2—N1—C3	56.9 (7)
Br1^{iv}—Pb1—Br1^{ii}	179.3 (7)	C2^{vii}—N1—C3^{vi}	127.8 (2)
Br1^{iv}—Pb1—Br1	83.6 (5)	C2^{vii}—N1—C3	127.8 (2)
Br1^{iv}—Pb1—Br1^{iii}	96.87 (6)	C2—N1—C3^{vii}	127.8 (2)
Br1^{i}—Pb1—Br1^{v}	179.3 (7)	C2^{vi}—N1—C3^{vi}	56.9 (7)
Br1^{i}—Pb1—Br1^{ii}	96.87 (6)	C2^{vii}—N1—C3^{vii}	56.9 (7)
Br1^{iv}—Pb1—Br1^{v}	96.87 (6)	C3—N1—C3^{vii}	99 (3)
Br1—Pb1—Br1^{ii}	96.87 (6)	C3—N1—C3^{vi}	99 (3)
Br1—Pb1—Br1^{v}	96.87 (6)	C3^{vi}—N1—C3^{vii}	99 (3)
Br1^{iii}—Pb1—Br1^{ii}	82.6 (5)	C1^{vii}—C1—C1^{vi}	60.000 (15)
Br1^{i}—Pb1—Br1^{iii}	96.87 (6)	C1^{vi}—C1—C2	111 (2)
Br1—Pb1—Br1^{iii}	179.3 (7)	C1^{vii}—C1—C2	111 (2)

Pb1—Br1—Pb1^{viii}	79.99 (8)	N1—C2—C1	93.9 (11)
C2^{vi}—N1—C2^{vii}	100 (3)	N1—C2—C3	71.6 (9)
C2^{vi}—N1—C2	100 (3)	C3—C2—C1	165.5 (16)
C2—N1—C2^{vii}	100 (3)	C2—C3—N1	51.5 (7)

Symmetry codes: (i) −*y*+1, *x*−*y*−1, *z*; (ii) *x*−*y*, *x*−1, *z*+1/2; (iii) −*x*+2, −*y*, *z*+1/2; (iv) −*x*+*y*+2, −*x*+1, *z*; (v)