Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

Influence of the organic cation disorder on photoconductivity in ethylenediammonium lead iodide, $NH_3CH_2CH_2NH_3PbI_4$

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Powder XRD characteristics

XRD profile of a flake-shaped phase (Fig.S1(a)) can be fitted by le-Bail decomposition with the monoclinic unit cell parameters a = 21.82425, b = 15.29009, c = 34.49222 Å and β = 96.3269°. XRD profile of the cube-shaped phase (Fig.S1(b)) has been fitted by the Rietveld refinement of the model obtained from the single crystal structure determination of the titled, $NH_3CH_2CH_2NH_3PbI_4$, compound.

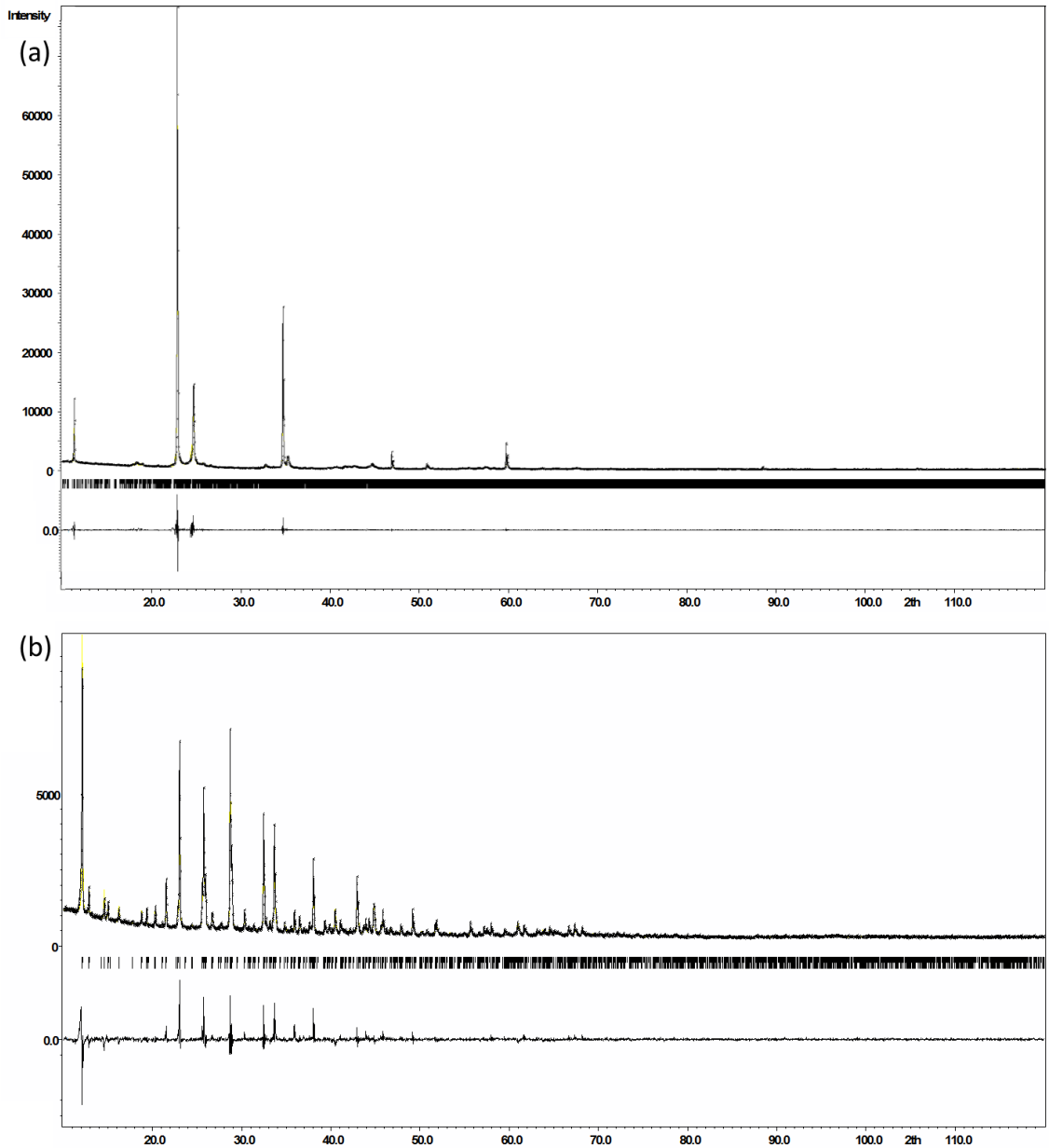

Figure S1 Powder XRD profiles of two simultaneously obtained phases: (a) a flake-shaped phase, (b) a cube-shaped phase.

Chemical composition

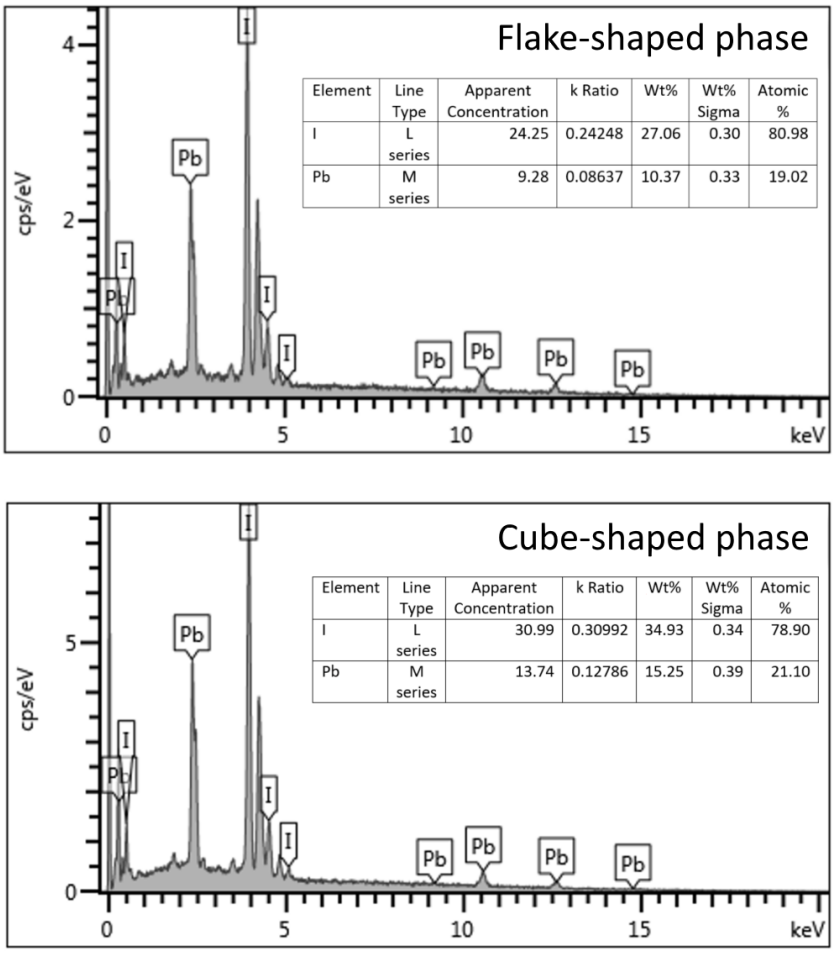

Figure S2 EDX spectra of the different phases of $NH_3CH_2CH_2NH_3PbI_4$ crystal. From the analysis can be seen that both phases have lead to iodine ratio 1:4.

Thermogravimetric analysis

The analysis were done on a Perkin Elmer TGA 4000 system with an auto sampler. TGA of both phases were done in N_2 atmosphere, the temperature program was from 313 K to 573 K with a heating rate of 10K/min and the sample was kept at 573 K for 20 minutes.

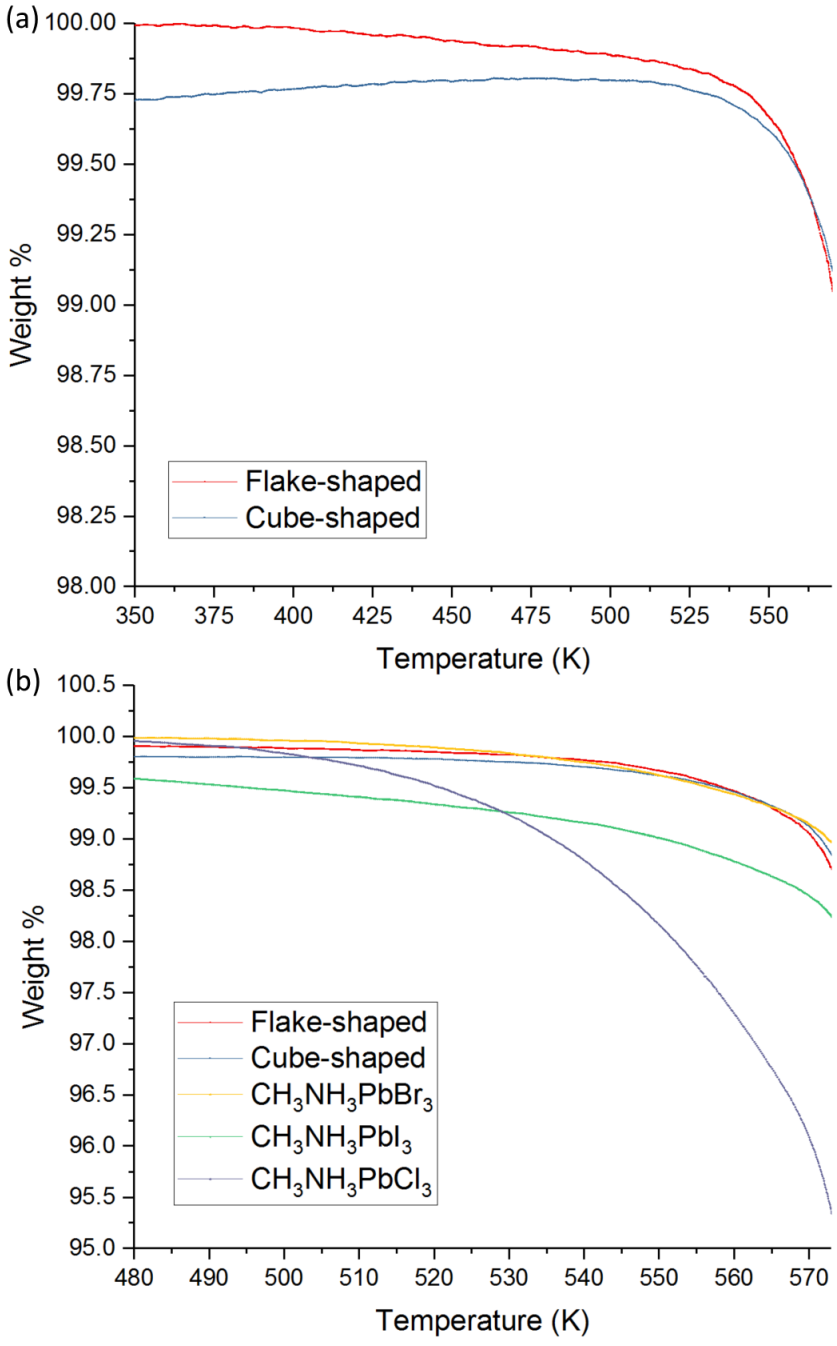

Figure S3 TGA of the flake-shaped and cube-shaped phases (a); Comparison with TGA of well-studied $CH_3NH_3PbI_3$, $CH_3NH_3PbBr_3$, $CH_3NH_3PbCl_3$ crystals.

Reference information on J-V curves

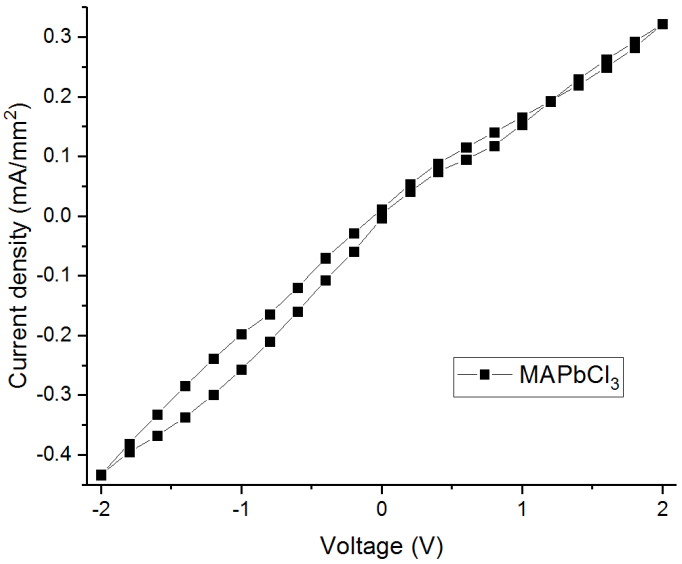

Figure S4 J-V curves of $CH_3NH_3PbCl_3$ under UV illumination (365 nm) with an intensity of 0.055 $mWmm^{-2}$.

Crystal structure information

Table S1 Selected interatomic distances (Å) and angles (deg.) in the pristine and the thermally treated crystals

	Pristine	Thermally treated
Distances in PbI_6 octahedra		
Pb1 - I3	3.2176(19)	3.208(4) x6
Pb2 - I4	3.200(2)	3.197(7) x6
Pb3 - I2	3.118(2)	3.130(6) x3
- I3	3.355(2)	3.353(5) x3
Pb4 - I1	3.110(2)	3.087(5) x3
-I4	3.374(2)	3.376(6) x3
Distances in ED cation		
N1 - C1	1.432(15)	(a) 1.41(4); (b) 1.41(6)
C1 - C2	1.445(13)	(a) 1.43(5); (b) 1.43(5)
C2 - N2	1.508(16)	(a) 1.52(4); (b) 1.52(5)
Angles in ED cation		
N1 - C1 - C2	115.5(10)	113.6(19)
C1 - C2 - N2	112.7(9)	117.5(16)
O - I distances		
O1 - I1	3.23(4) x3	None
O1 - I2	None	3.22(4) ×3

Table S2 H-bond characteristics (Å, °) for the pristine and thermally treated crystals

	D-H	H...*A*	*D*...*A*	*D*-H...*A*
Pristine				
N1-H1n1...I2	0.96	2.85	3.659(9)	142.27
N1-H3n1...I2	0.96	2.66	3.521(12)	149.76
N2-H1n2...I1	0.96	2.64	3.511(15)	151.37
N2-H2n2...I1	0.96	2.65	3.586(18)	163.71
N2-H3n2...I1	0.96	2.78	3.592(11)	142.61
Thermally treated				
Split cation model				
N1a-H1n1a...I2	0.96	2.71	3.48(2)	137.72
N2a-H1n2a...I3	0.96	2.83	3.63(3)	141.03
N2a-H3n2a...I1	0.96	2.70	3.58(6)	153.73
N2a-H2n2a...I1	0.96	2.49	3.39(7)	155.59
N1b-H2n1b...I2	0.96	2.82	3.54(4)	132.43
N2b-H1n1b...I1	0.96	2.76	3.60(10)	146.69
N2b-H3n1b...I1	0.96	2.84	3.62(8)	138.99