Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

Anomalous inclusion of chloride ions in ethylenediammonium lead iodide turns 1D non-perovskite to 2D perovskite structure

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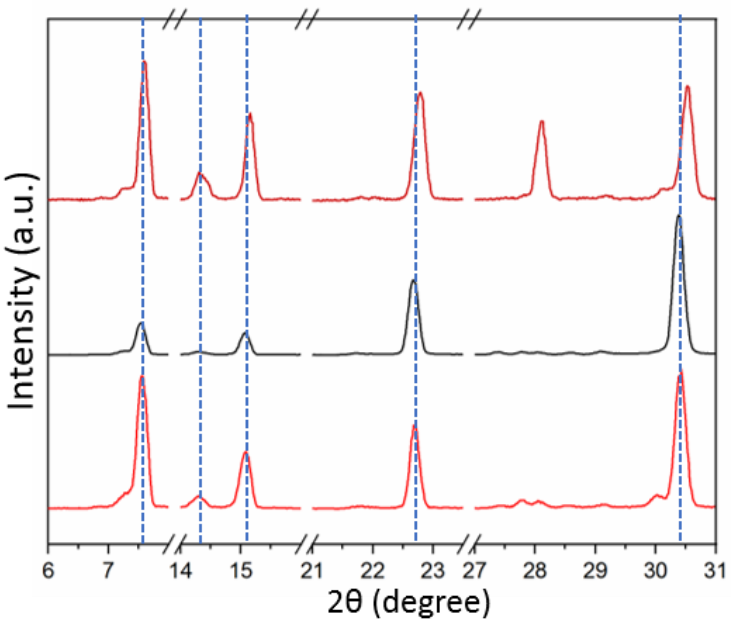

Figure S1. Close-up views of the XRD patterns of $[(ED)_2PbI_4]Cl_2$ (red), CC-$[(ED)_2PbI_4]Cl_2$ (black), and the sample obtained from heating the colour-changed crystals at 100°C (dark red)

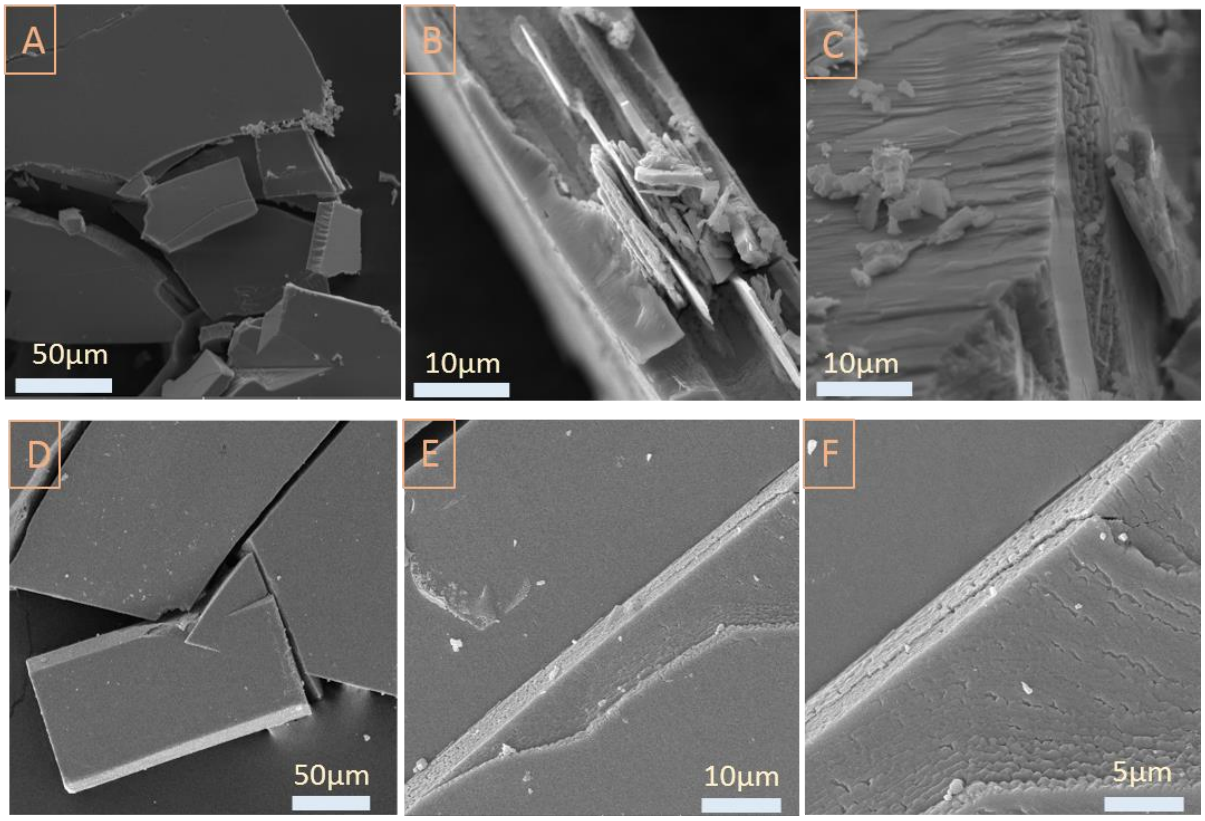

Figure S2. FESEM images at different magnifications for $[(ED)_2PbI_4]Cl_2$ (A, B, C) and CC-$[(ED)_2PbI_4]Cl_2$ (D, E, F)

Table S1. Crystallographic data of $EDPbI_4$ and $[(ED)_2PbI_4]Cl_2$

	$EDPbI_4$[1]	$[(ED)_2PbI_4]Cl_2$
Empirical formula	$C_2H_{10}N_2O_{0.042(4)}PbI_4$	$C_4H_{20}N_4PbI_4Cl_2$
Formula weight (g/mol)	777.60	909.94
Space group	$R\bar{3}$	Pbcm
a, Å	14.5906(1)	8.7590(4)
b, Å	14.5906(1)	9.4400(4)
c, Å	32.7775(5)	23.5450(8)
α, °	90	90
β, °	90	90
γ, °	120	90
Z	18	4
V, $Å^3$	6043.00(14)	1946.82(14)
ρ(g/cm^3)	-	3.105

Table S2. Observed FTIR Wavenumbers(cm^{-1}) and band assignments

Observed wavenumbers(cm^{-1})				**Assigned to**
en. 2HI	**$EDPbI_4$**	**$[(ED)_2PbI_4]Cl_2$**	**Color-changed $[(ED)_2PbI_4]Cl_2$**	
3142	3064	3090	3091	NH_3 asymmetric stretching
2999	3006	2989	2990	NH_3 symmetric stretching
2912	2925	2920	2920	CH_2 asymmetric stretching
2785	2880	2850	2850	CH_2 symmetric stretching
1627	1643	1644	1643	NH_3 asymmetric deformation
1560	1549	1563	1560	NH_3 symmetric deformation
1491	1464	1481	1481	CH_2 scissoring
1348	-	1439	1439	CH_2 wagging
1311	1317	1307	1307	CH_2 twisting
-	1177	1154	1155	NH_3 rocking
1026	1026	1019	1018	CN stretching
997	994	957	957	NH_3 rocking
914	875	887	887	CH_2 rocking
787	765	806	806	CH_2 rocking
548,465	460	464	464	^+N-C-C-N^+ bending

Theoretical calculation of weight loss percentage:

The calculation was performed as follows:

For each crystal, we assumed that the following species (listed in Table S3) can remove from the structure. Based on the molecular weight (Mw) of the crystals (according to the Table S1) and Mw of the considered species, the weight loss percentages were calculated. By comparing the loss percentage values obtained from TGA analysis with those calculated theoretically we determined the possible decomposed fragments.

Table S3. Theoretical weight loss percentages for $EDPbI_4$ and $[(ED)_2PbI_4]Cl_2$ crystals

Crystal formula	Considered fragment	Mw of the fragment (Mw_f, gr/mol)	Theoretical weight loss percentage $(\frac{Mwf}{Mwcrystal})\times 100$
$EDPbI_4$	ED+ 2I	315.92	40.63%
$[(ED)_2PbI_4]Cl_2$	2(ED)+ 2I+2Cl	448.94	49.34%
	2(ED)+ 3I+ Cl	540.39	59.39%
	2(ED)+ 4I	631.85	69.44%

References:

[1] A. Glushkova, A. Arakcheeva, P. Pattison, M. Kollár, P. Andričević, B. Náfrádi, L. Forró and E. Horváth, *CrystEngComm*, 2018, **20**, 3543