Electronic Supplementary Material (ESI) for ChemComm.

A Facile Solvo-Thermal Growth of Single Crystal Mixed Halide Perovskite $CH_3NH_3Pb(Br_{1-x}Cl_x)_3$

Supporting Information:

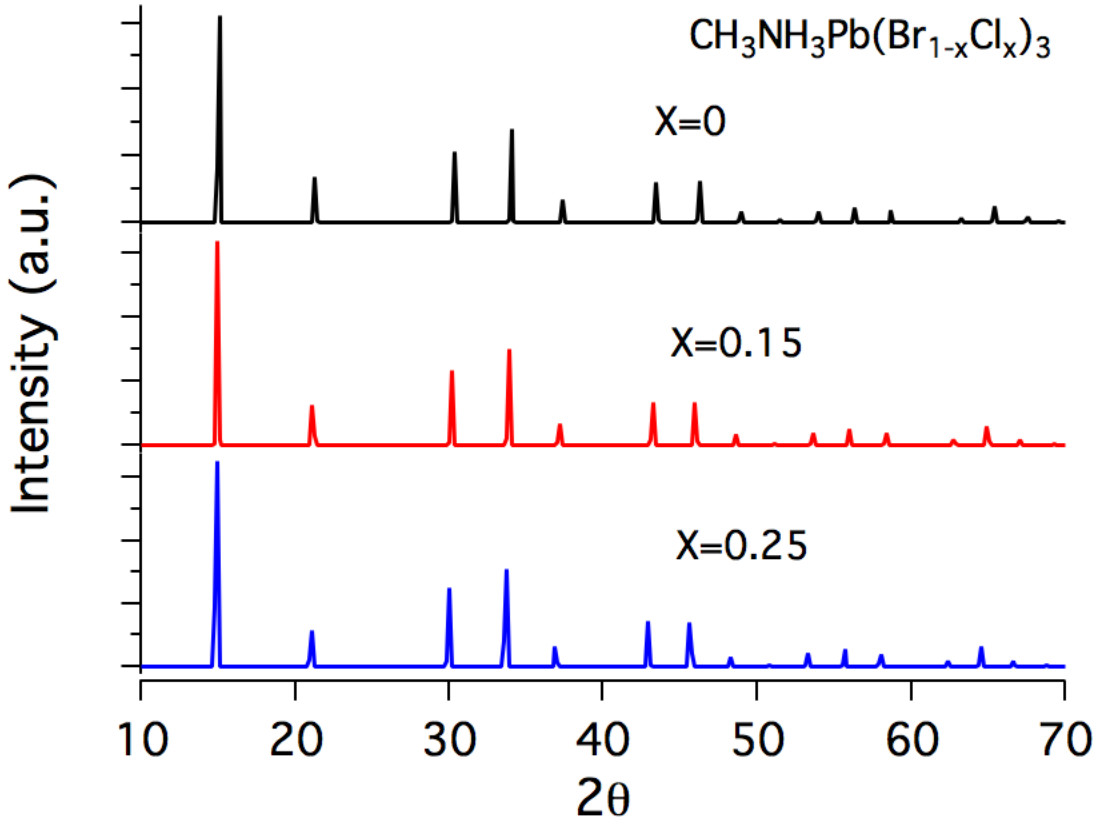

Figure S1. Simulated XRD patterns of $CH_3NH_3Pb(Br_{1-x}Cl_x)_3$ (x=0, 0.15 and 0.25) perovskites single crystals

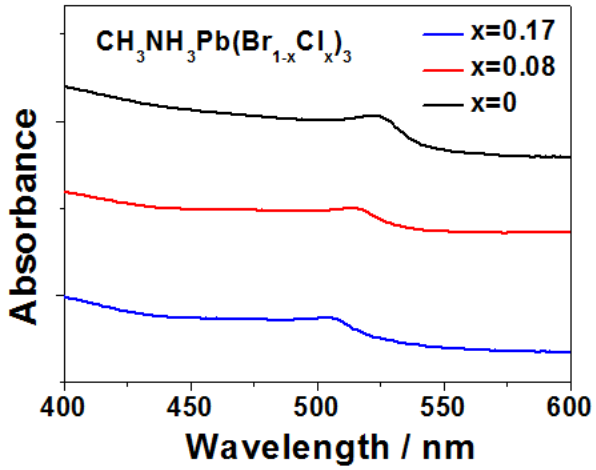

Figure S2. UV-vis spectra of thin films of $CH_3NH_3Pb(Br_{1-x}Cl_x)_3$ perovskites prepared from the precursor solutions of [$PbBr_2$ + (1-y) CH_3NH_3Br+ yCH_3NH_3Cl] (y=0, 0.25 and 0.5), corresponding to the Cl/(Cl+Br) ratios of about 0, 0.08, and 0.17, respectively.

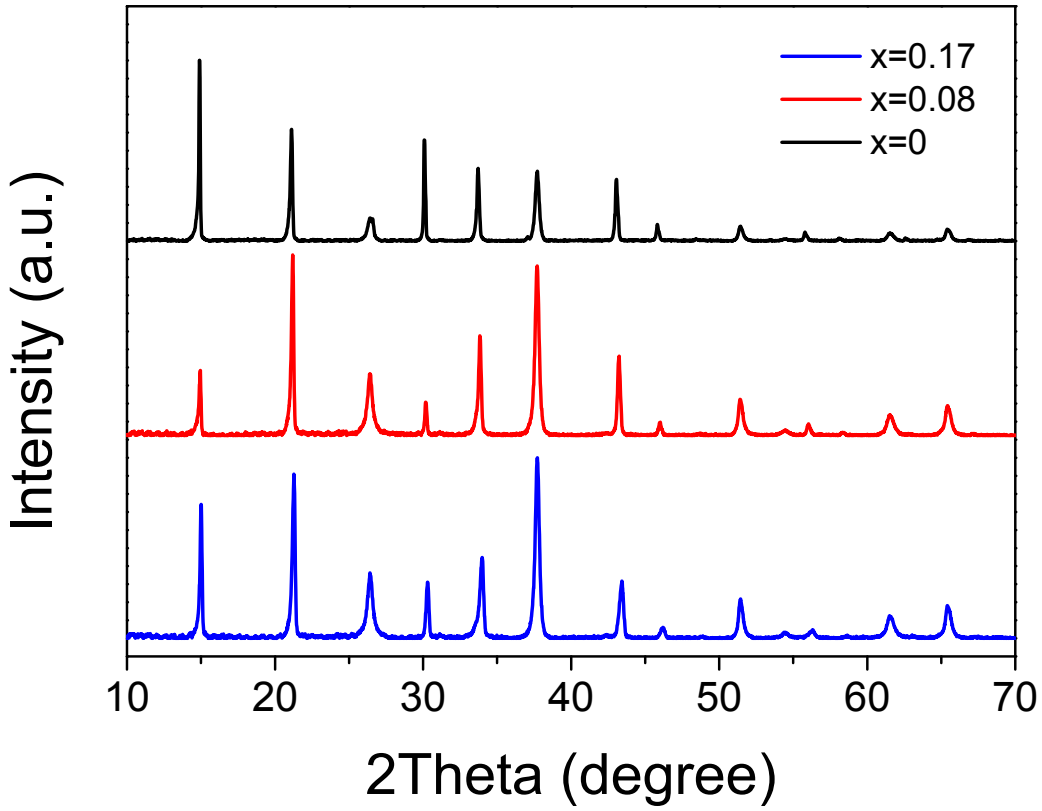

Figure S3. XRD patterns of thin films of CH3NH3Pb(Br1-xClx)3 perovskites prepared from the precursor solutions of [PbBr2 + (1-y) CH3NH3Br+ yCH3NH3Cl] (y=0, 0.25 and 0.5), corresponding to the Cl/(Cl+Br) ratios of about 0, 0.08, and 0.17, respectively.

Table S1. Calculated total energies for various systems

System	Total energy (eV)
MABr + MACl + $PbBr_2$	-95.948
$MAPbBr_3$ + MACl	-96.101
$MAPbBr_2Cl$ + MABr	-96.142
MAI + MACl+PbI_2	-94.306
$MAPbI_3$ + MACl	-94.307
$MAPbI_2Cl$ + MAI	-94.110

X-ray structure determination.

Single crystal X-ray diffraction studies were carried out a Bruker Apex II CCD-based X-ray diffractometer equipped with Mo *K*α radiation (λ = 0.71073 Å). The crystals were mounted on a on fine glass fibers with otime, and data was collected at room temperature using ω and ϕ scans. Data was integrated using the Bruker SAINT software program and scaled using the SADABS software program. Using Olex2[1], the structure was solved with the SHELXTL software suite[2] using Direct Methods and refined by full-matrix Least Squares minimisation[3]. Due to crystallographic disorder of the methylamonium cation the corresponding electron density was removed using the *SQUEEZE* routine of *PLATON*.[4] Crystallographic data is summarized in Table S2.

Table S2. Crystallographic Data and Refinement Information

Compound	**$CH_3NH_3PbBr_3$**	**$CH_3NH_3Pb(Br_{0.85}Cl_{0.15})_3$**	**$CH_3NH_3Pb(Br_{0.75}Cl_{0.25})_3$**
empirical formula	$C_2H_6N_1Br_3Pb_1$	$C_2H_6N_1Cl_{0.45}Br_{2.55}Pb_1$	$C_2H_6N_1Cl_{0.75}Br_{2.25}Pb_1$
formula weight	490.99	470.98	457.63
crystal system	Cubic	Cubic	Cubic
lattice parameters			
$a = b = c$ (Å)	5.9312(3)	5.8959(4)	5.8638(7)
$\alpha = \beta = \gamma$ (deg)	90	90	90
V (Å^3)	208.65(3)	204.95(4)	201.62(7)
space group	*P*m-3m	*P*m-3m	*P*m-3m
Z value	1	1	1
Density calc (g/cm3)	3.554	3.664	3.395
Wavelength (Å)	0.71073	0.71073	0.71073
temperature (K)	293(2)	293(2)	293(2)
2θ max (°)	54.80	55.16	54.97
no. obs. [$I > 2$ sigma (I)]	74	74	72
no. parameters	5	5	5
goodness of fit on F^2	1.493	1.307	1.396
max. shift in cycle	0.000	0.000	0.000
residuals: R_1; wR_2	0.0187; 0.0552	0.0230; 0.0565	0.0396; 0.1019
largest peak	0.595	0.598	1.252
deepest hole	-0.809	-0.703	-0.943

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
2. G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3-8.
3. G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112-122.
4. P. v. d. Sluis and A. L. Spec, *Acta Cryst.*, 1990, **A46**, 194-201.