Supporting Information

A Powder XRD, Solid State NMR and Calorimetric Study of the Phase Evolution in Mechanochemically Synthesized Dual Cation $(Cs_x(CH_3NH_3)_{1-x})PbX_3$ Lead Halide Perovskite Systems†‡

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KEYWORDS: Mechanochemical synthesis, hybrid lead halide perovskites, multinuclear solid state NMR, phase evolution, chemical shielding, cesium-methylammonium miscibility.

† The experimental data for this study are provided as a supporting dataset from WRAP, the Warwick Research Archive Portal at http://wrap.warwick.ac.uk/160750/

‡ Electronic supplementary information (ESI) available: Supporting experimental and materials characterization including HRTEM, ^{207}Pb MAS NMR data, high resolution laboratory source powder XRD data for the Cl series and Br series, DSC data, UV/vis data with Tauc plots, in addition to tables summarising the ^{133}Cs, ^{207}Pb and ^{1}H T_1 (spin-lattice) relaxation times and the variable temperature evolution of refined lattice parameters for each system. See DOI:10.1039/XXXXXXXX.

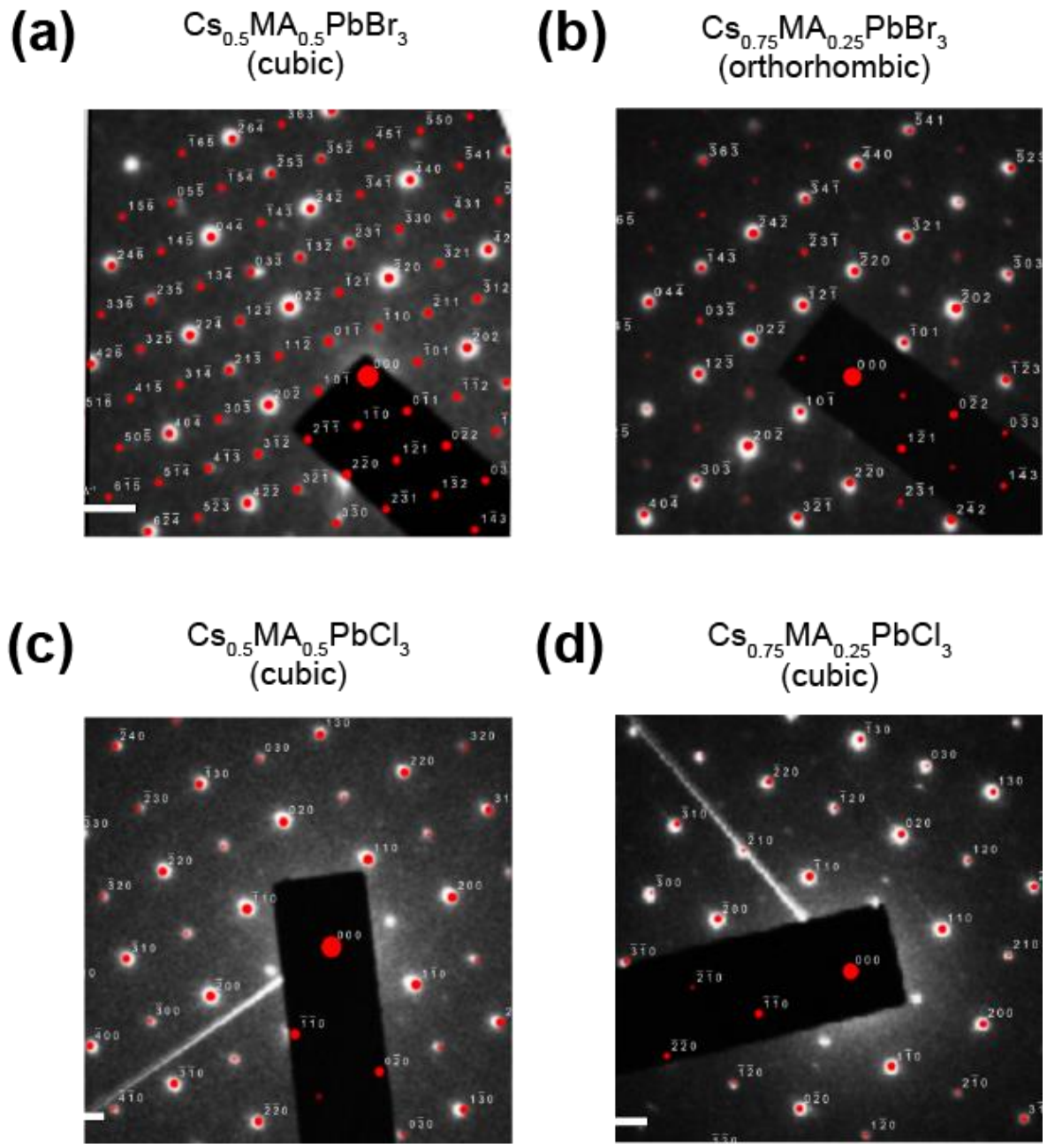


Figure S1. Indexed selected area electron diffraction (SAD) patterns of selected powder samples prepared under mechanochemical conditions.

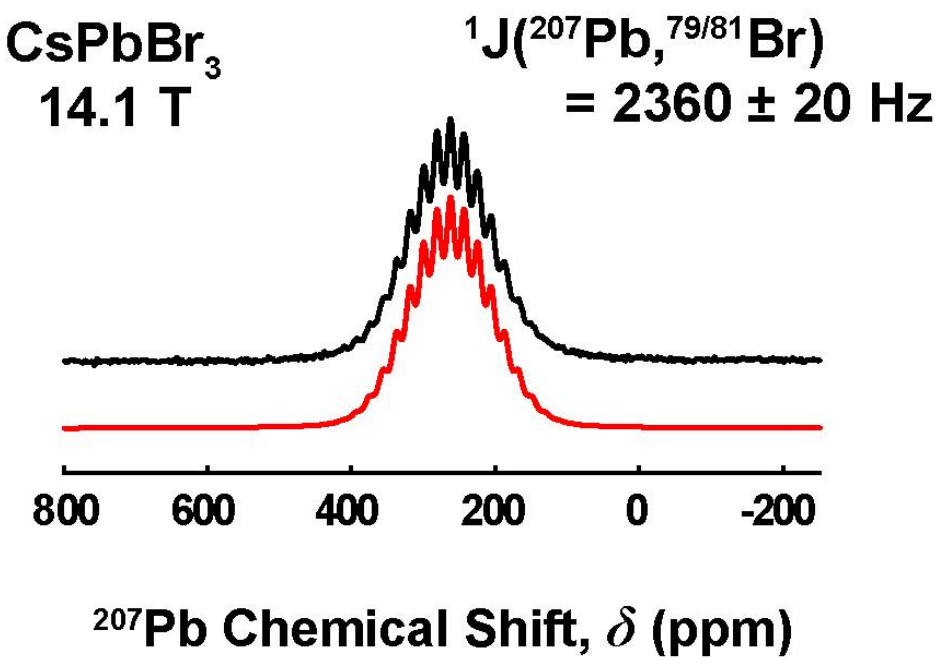
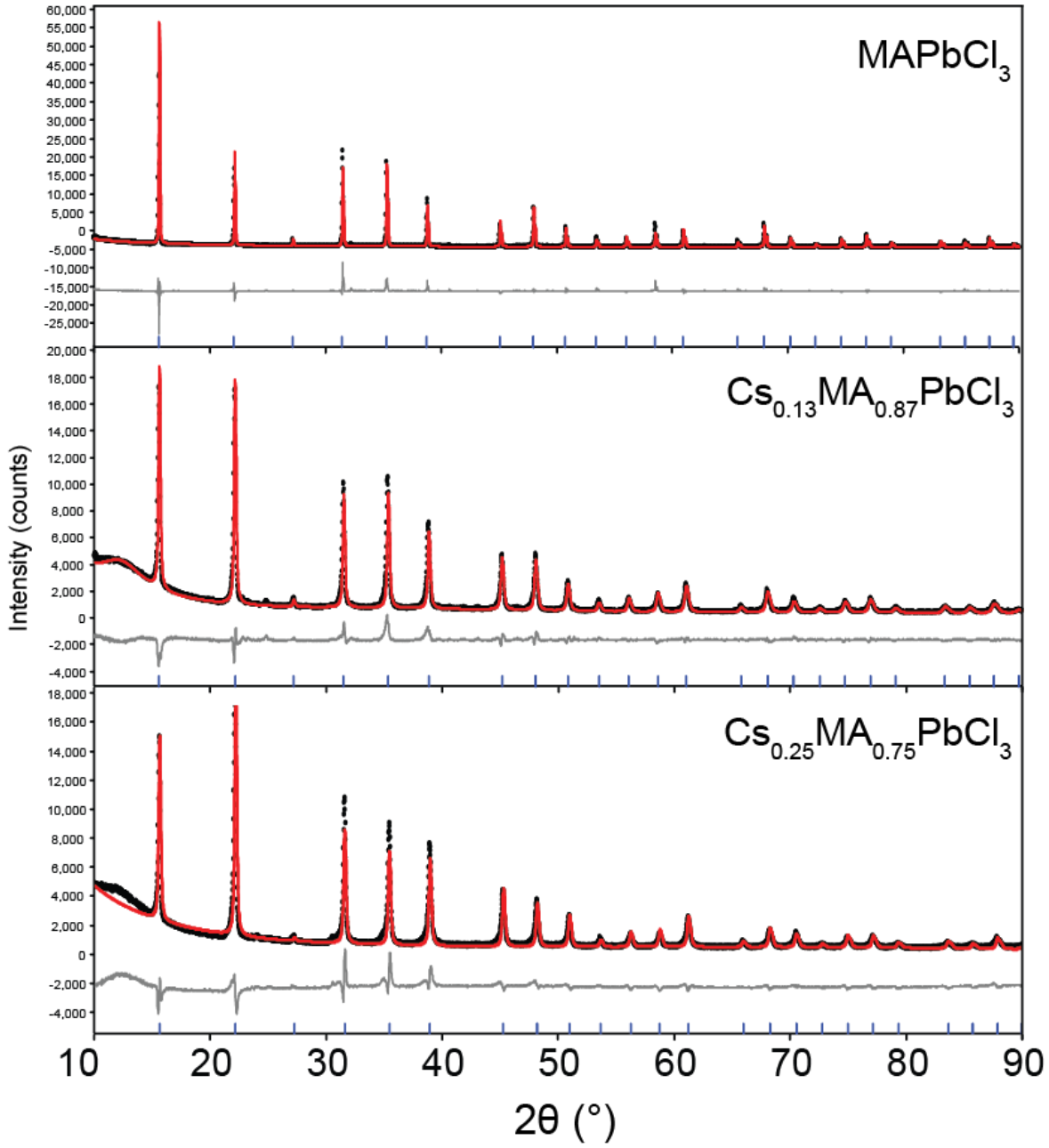
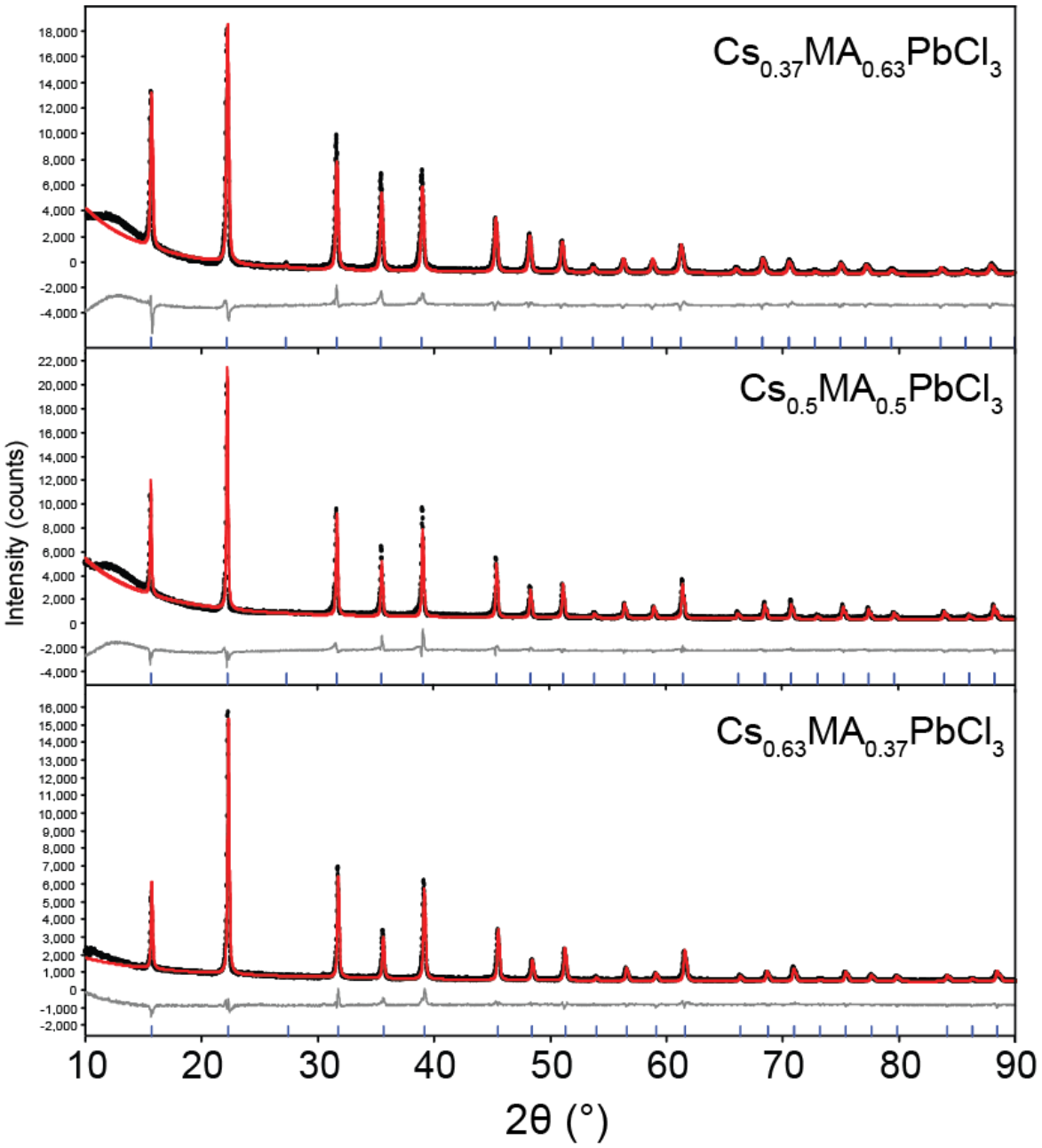


Figure S2. A simulation of the ^{1}J(Pb,Br) coupling observed on the ^{207}Pb MAS NMR data from $CsPbBr_3$ measured at 14.1 T. This simulation was undertaken using the DMFiT software package and a ^{1}J(Pb,Br) coupling constant of 2360 ± 20 Hz was measured.


MAPbCl3
Cs0.13MA0.87PbCl3
Cs0.25MA0.75PbCl3
Intensity (counts)
2θ (°)
10
20
30
40
50
60
70
80
90


Cs0.37MA0.63PbCl3
Cs0.5MA0.5PbCl3
Cs0.63MA0.37PbCl3
Intensity (counts)
2θ (°)

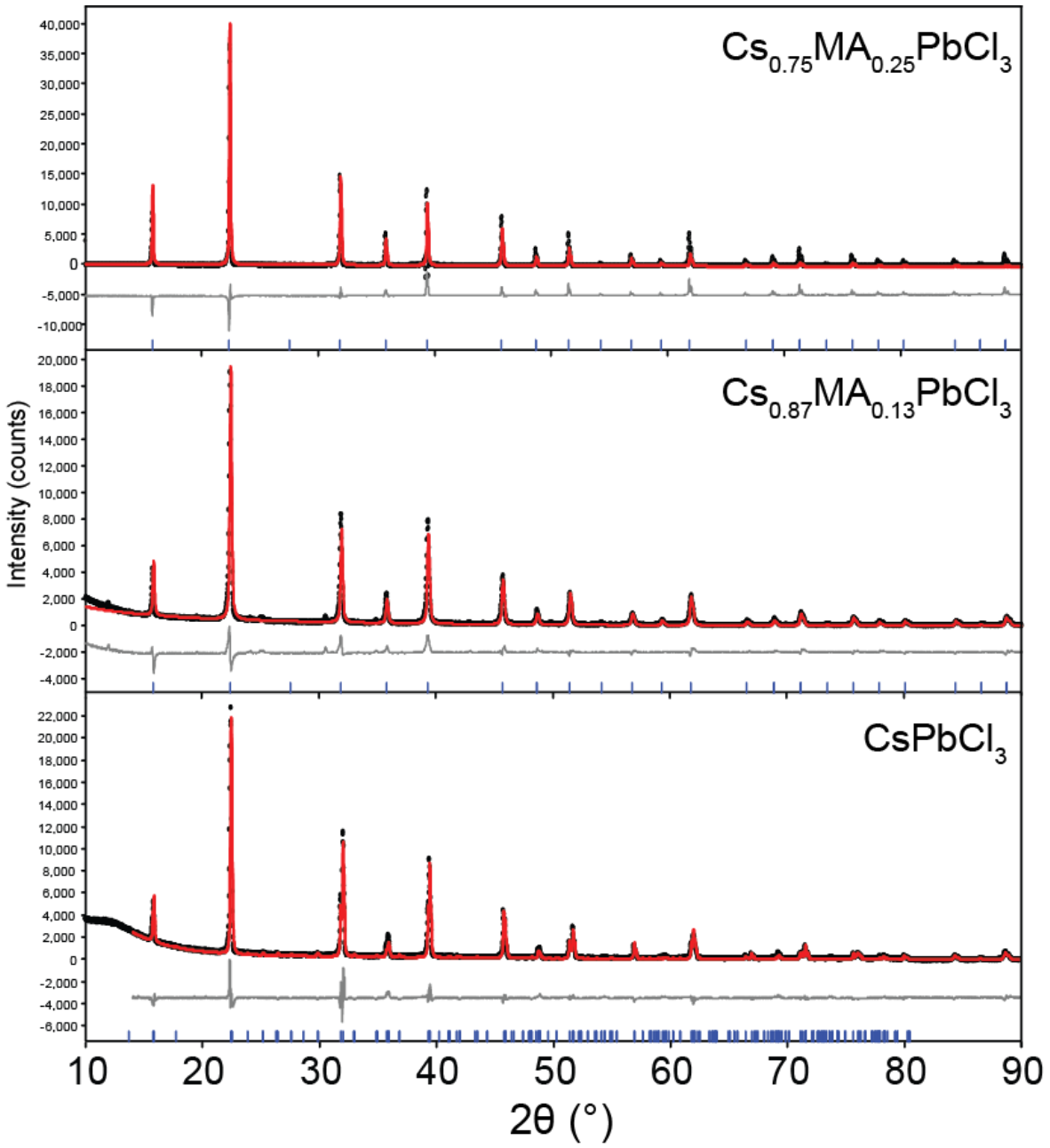
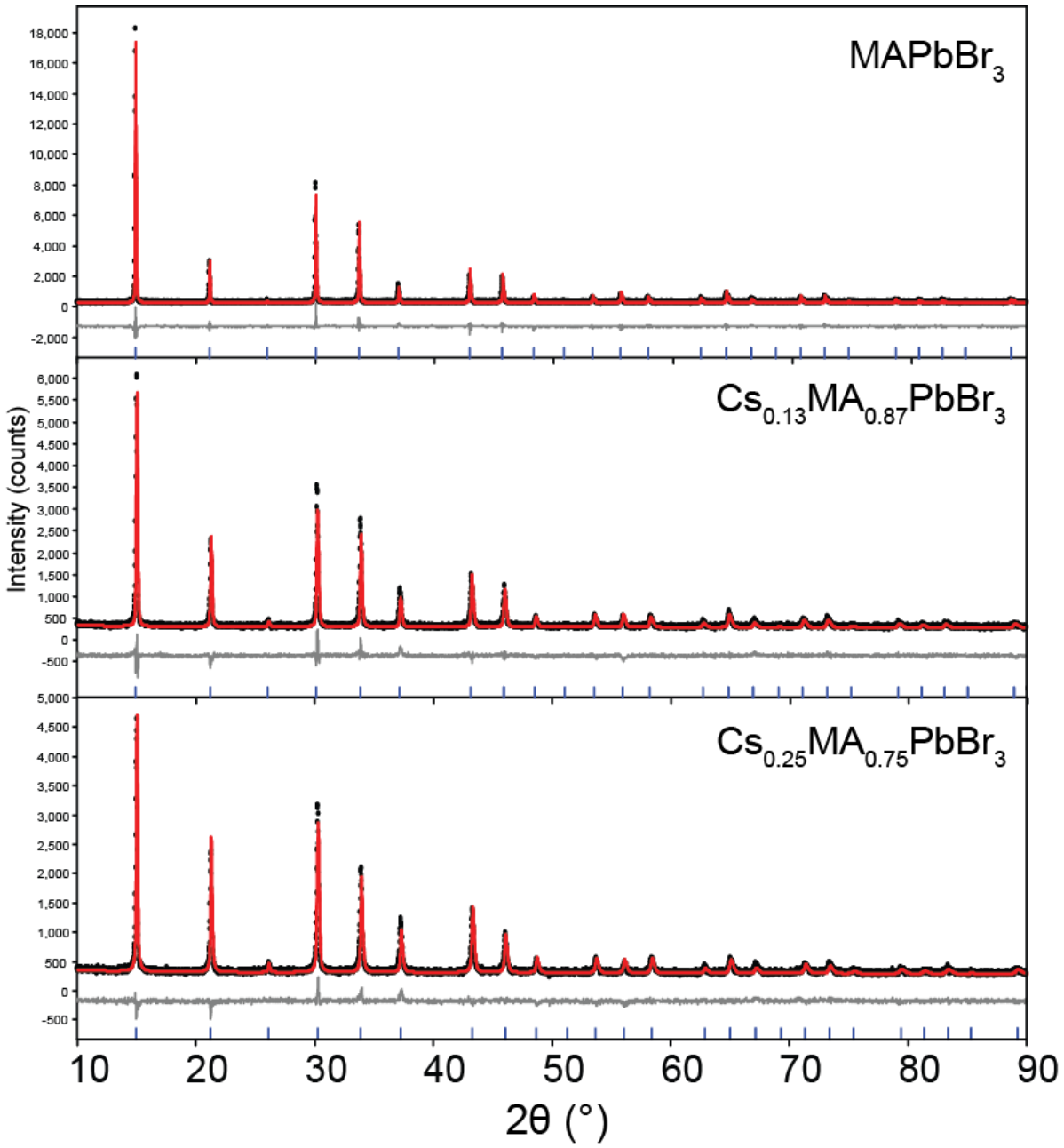
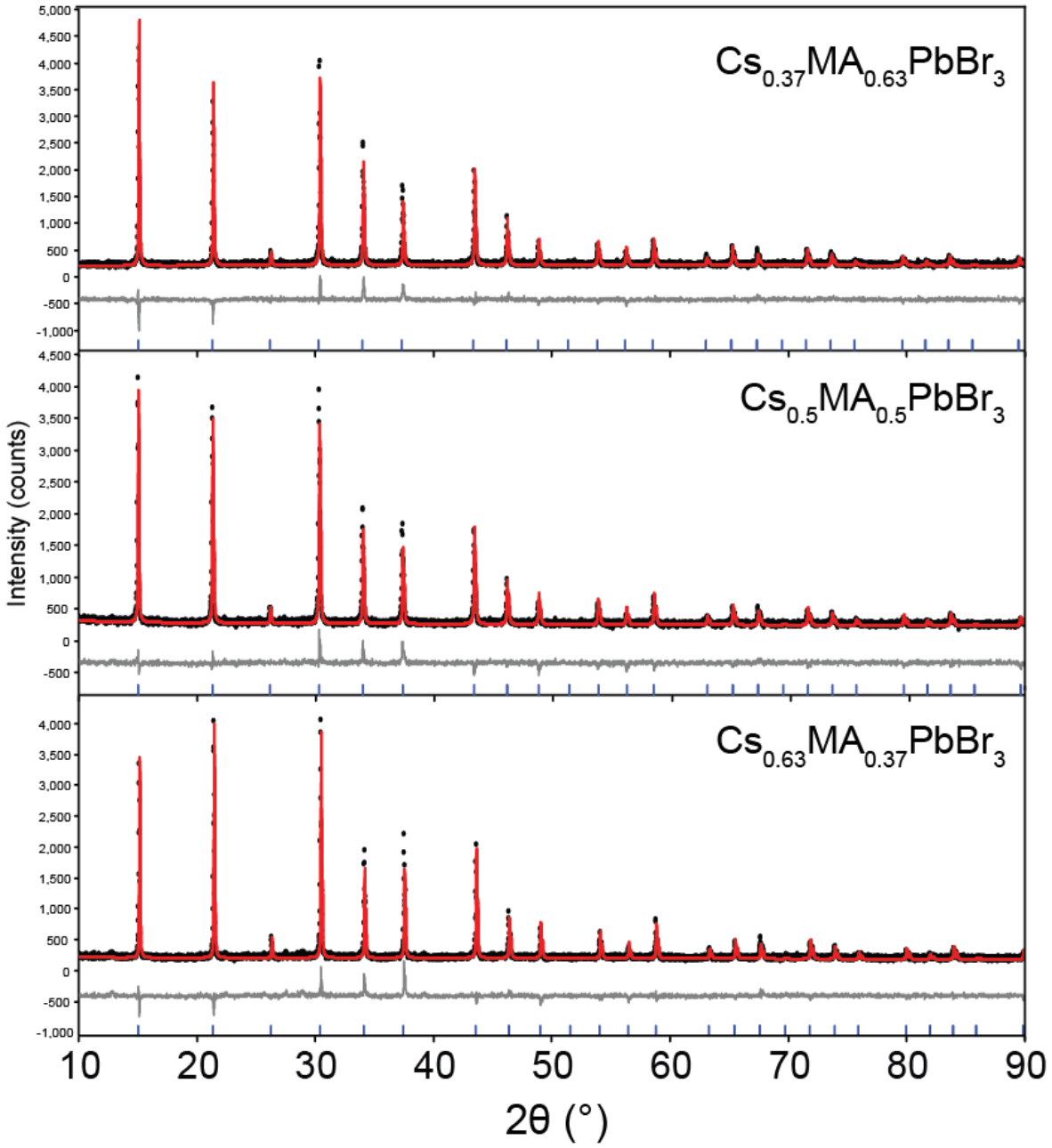


Figure S3. Room temperature high resolution laboratory source PXRD data and Rietveld refinement fits from the $Cs_xMA_{1-x}PbCl_3$ (x = 0 - 1) solid solution series.


MAPbBr3
Cs0.13MA0.87PbBr3
Cs0.25MA0.75PbBr3
Intensity (counts)
2θ (°)
10
20
30
40
50
60
70
80
90


Cs0.37MA0.63PbBr3
Cs0.5MA0.5PbBr3
Cs0.63MA0.37PbBr3
Intensity (counts)
2θ (°)
10
20
30
40
50
60
70
80
90

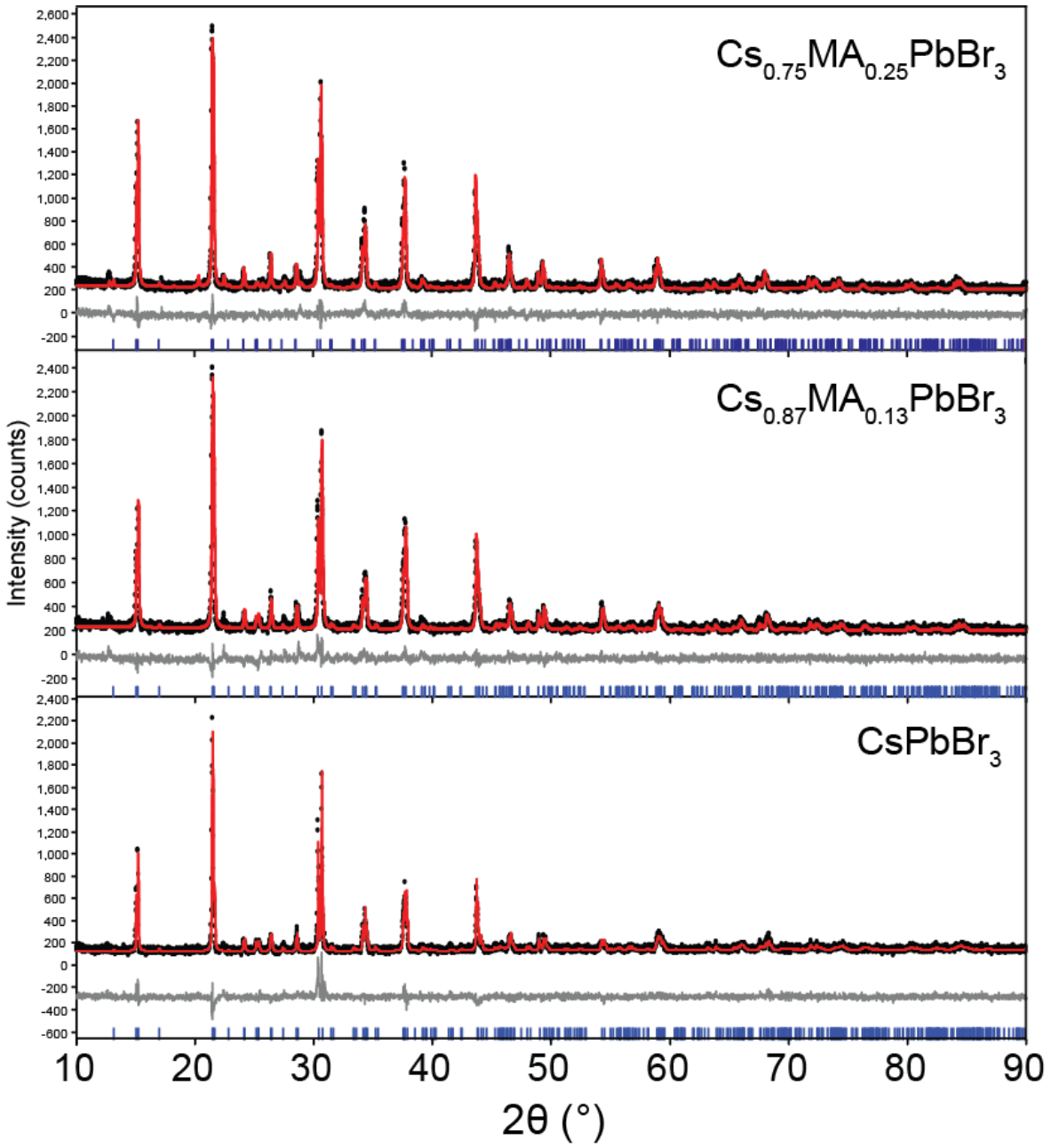


Figure S4. Room temperature high resolution synchrotron PXRD data and Rietveld refinement fits from the $Cs_xMA_{1-x}PbBr_3$ (x = 0 - 1) solid solution series.

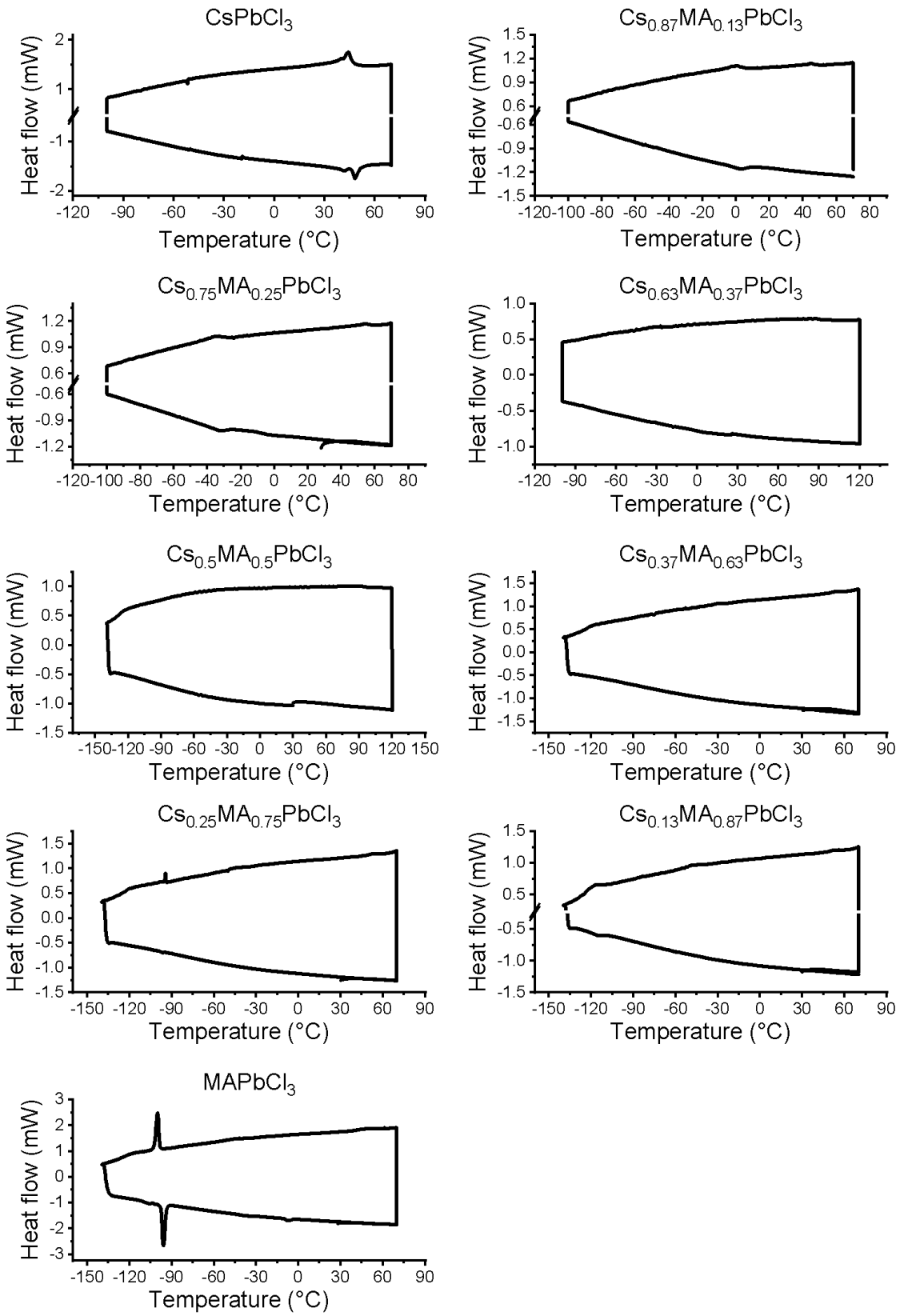


Figure S5. DSC data from the $(Cs_xMA_{1-x})PbCl_3$ solid solution series showing phase transitions involving a change in latent heat.

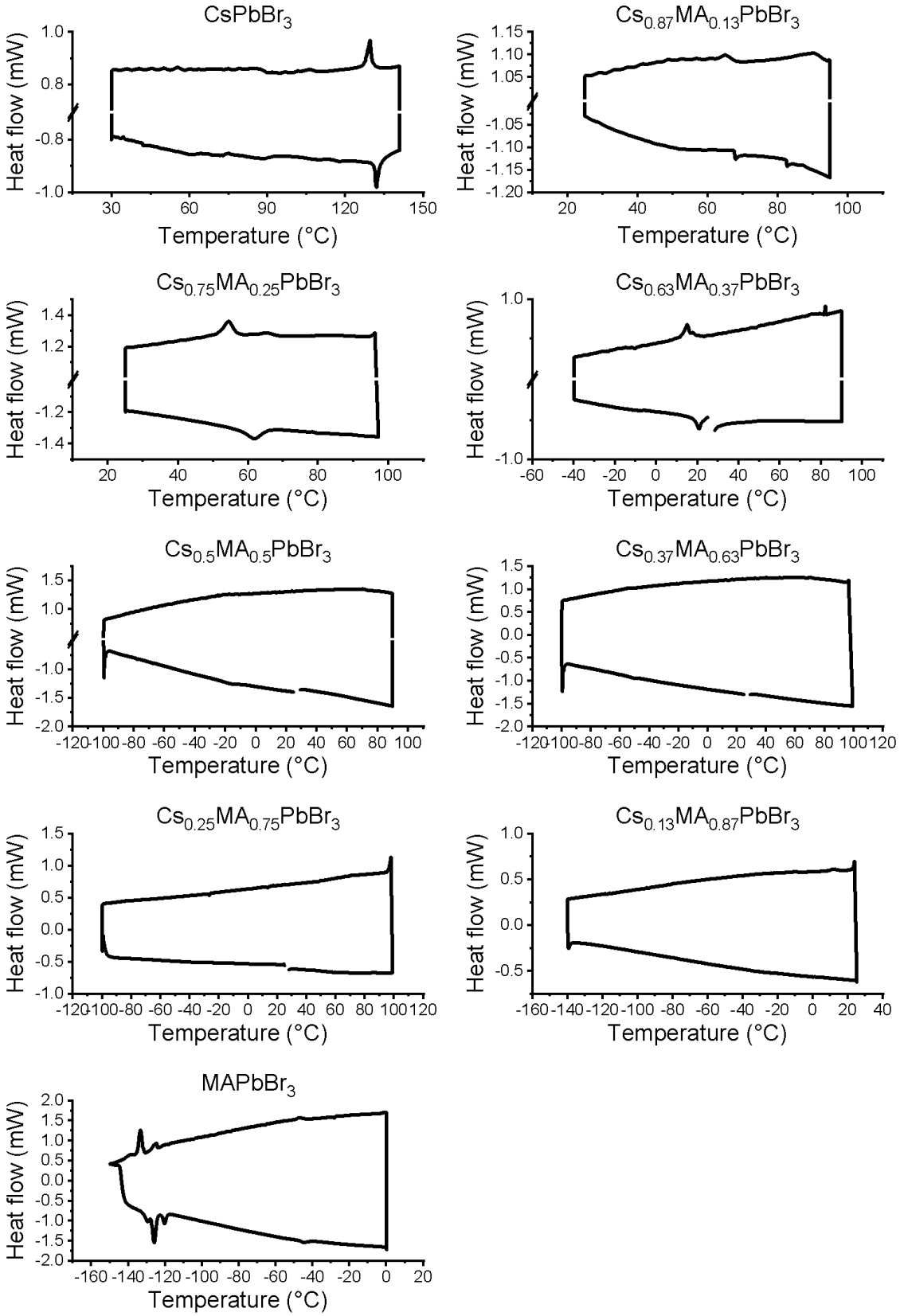


Figure S6. DSC data from the $(Cs_xMA_{1-x})PbBr_3$ solid solution series showing phase transitions involving a change in latent heat.

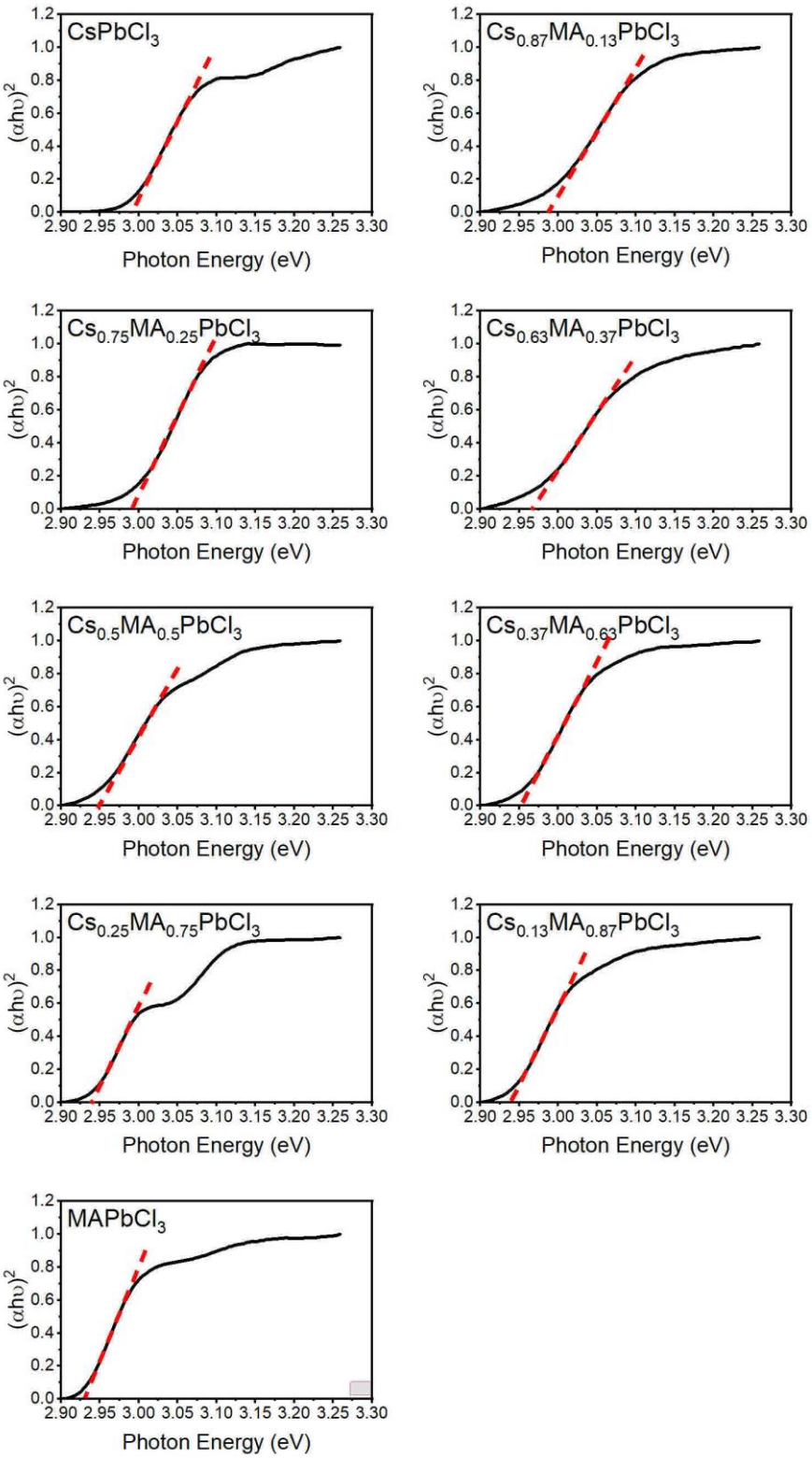


Figure S7. Tauc plots from the UV/vis data from the $(Cs_xMA_{1-x})PCl_3$ (x = 0 - 1) solid solution series enabling a determination of the bandgap variation across each system.

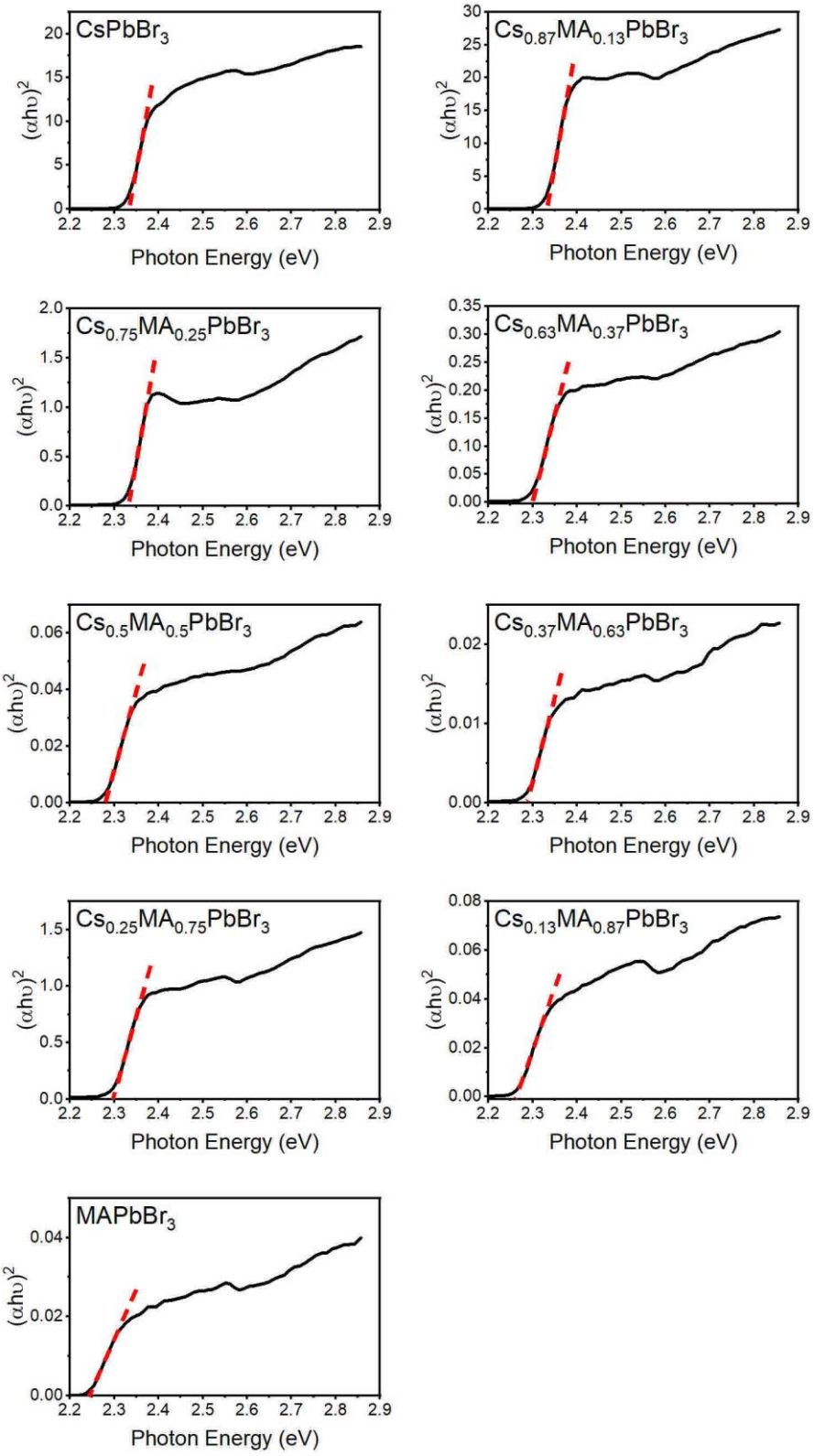


Figure S8. Tauc plots from the UV/vis data from the $(Cs_xMA_{1-x})PBr_3$ (x = 0 - 1) solid solution series enabling a determination of the bandgap variation across each system.

Table S1. The ^{133}Cs, ^{207}Pb and ^{1}H T_1 (spin-lattice) relaxation times as measured by the saturation-recovery method.

Nominal composition	^{133}Cs T_1 (s)	^{207}Pb T_1 (s)	^{1}H T_1 (s)
$MAPbBr_3$	-	1.3 (± 0.3)	18.3 (± 3.7)
$Cs_{0.13}MA_{0.87}PbBr_3$	47.0 (± 9)	2.2 (± 0.4)	5.7 (± 1.1)
$Cs_{0.25}MA_{0.75}PbBr_3$	32.6 (± 6)	1.2 (± 0.2)	3.5 (± 0.7)
$Cs_{0.37}MA_{0.63}PbBr_3$	24.5 (± 5)	2.9 (± 0.6)	4.9 (± 1.0)
$Cs_{0.50}MA_{0.50}PbBr_3$	14.5 (± 3)	3.2 (± 0.6)	3.3 (± 0.7)
$Cs_{0.63}MA_{0.37}PbBr_3$	8.1 (± 2)	5.0 (± 1.0)	2.9 (± 0.6)
$Cs_{0.75}MA_{0.25}PbBr_3$	17.4 (± 3)	3.5 (± 0.7)	1.4 (± 0.3)
$Cs_{0.87}MA_{0.13}PbBr_3$	21.8 (± 4)	5.9 (± 1.2)	2.1 (± 0.4)
$CsPbBr_3$	54.2 (± 10)	5.4 (± 1.1)	-
$MAPbCl_3$	-	1.6 (± 0.3)	7.1 (± 1.4)
$Cs_{0.13}MA_{0.87}PbCl_3$	43.5 (± 8.7)	1.1 (± 0.2)	0.9 (± 0.2)
$Cs_{0.25}MA_{0.75}PbCl_3$	34.4 (± 6.9)	1.3 (± 0.3)	1.0 (± 0.2)
$Cs_{0.37}MA_{0.63}PbCl_3$	28.3 (± 5.7)	1.4 (± 0.3)	0.8 (± 0.2)
$Cs_{0.50}MA_{0.50}PbCl_3$	29.8 (± 6.0)	1.5 (± 0.3)	2.5 (± 0.5)
$Cs_{0.63}MA_{0.37}PbCl_3$	16.0 (± 3.2)	1.5 (±0.3)	1.0 (± 0.2)
$Cs_{0.75}MA_{0.25}PbCl_3$	16.7 (± 3.3)	1.5 (±0.3)	2.7 (± 0.5)
$Cs_{0.87}MA_{0.13}PbCl_3$	8.0 (± 1.6)	1.5 (±0.3)	1.3 (± 0.3)
$CsPbCl_3$	50.8 (± 10.0)	1.7 (±0.3)	-

Table S2. Evolution of refined lattice parameters in $CsPbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
381.28	8.2676(1)	5.8901(9)	402.614(2)	1.93
383.15	8.2680(1)	5.8899(2)	402.635(0)	1.92
385.14	8.2687(2)	5.8896(4)	402.684(7)	1.92
387.18	8.2694(2)	5.8892(8)	402.728(9)	1.92
389.04	8.2702(4)	5.8890(0)	402.789(6)	1.92
391.02	8.2711(1)	5.8886(8)	402.851(3)	1.93
393.06	8.2720(6)	5.8882(0)	402.911(2)	1.95
394.80	8.2731(7)	5.8877(7)	402.990(4)	1.95
396.81	8.2741(1)	5.8872(9)	403.049(3)	1.97
398.66	8.2753(4)	5.8868(1)	403.136(5)	1.99
400.53	8.2765(9)	5.8862(4)	403.218(8)	2.03
402.24	8.2780(0)	5.8855(6)	403.309(8)	2.04
404.07	8.2796(2)	5.8847(4)	403.411(6)	2.07
405.98	8.2816(3)	5.8839(7)	403.554(1)	2.17
407.84	8.2835(2)	5.8829(5)	403.668(9)	2.21
409.93	8.2855(4)	5.8818(2)	403.787(6)	2.25
411.95	8.2872(1)	5.8805(9)	403.866(4)	2.26
413.48	8.2884(6)	5.8797(2)	403.928(2)	2.26
415.50	8.2897(0)	5.8787(5)	403.982(4)	2.26
417.50	8.2909(2)	5.8778(6)	404.040(6)	2.25
419.34	8.2919(9)	5.8771(8)	404.097(8)	2.31
421.24	8.2927(7)	5.8766(6)	404.138(3)	2.37
422.91	8.2936(3)	5.8763(1)	404.197(4)	2.44
425.05	8.2946(2)	5.8760(1)	404.273(2)	2.49
427.06	8.2954(0)	5.8756(8)	404.326(5)	2.51
428.97	8.2962(9)	5.8754(9)	404.400(8)	2.56
430.38	8.2970(7)	5.8753(3)	404.465(5)	2.59

Table S3. Evolution of refined lattice parameters in $Cs_{0.87}MA_{0.13}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
346.05	8.2694(7)	5.8934(6)	403.019(2)	1.83
348.03	8.2701(1)	5.8933(1)	403.071(9)	1.84
350.26	8.2708(1)	5.8931(1)	403.125(8)	1.82
352.15	8.2717(0)	5.8928(8)	403.197(0)	1.84
354.15	8.2725(9)	5.8926(1)	403.265(9)	1.83
356.12	8.2735(2)	5.8923(4)	403.337(0)	1.85
358.10	8.2744(6)	5.8919(8)	403.404(0)	1.85
360.00	8.2754(8)	5.8915(6)	403.474(3)	1.85
361.69	8.2765(1)	5.8911(9)	403.550(3)	1.87
363.56	8.2776(3)	5.8907(8)	403.631(4)	1.88
365.43	8.2788(8)	5.8902(7)	403.717(8)	1.88
367.50	8.2801(6)	5.8895(3)	403.792(4)	1.90
369.45	8.2817(6)	5.8889(5)	403.908(9)	1.95
371.31	8.2834(2)	5.8881(8)	404.017(8)	1.98
373.06	8.2850(0)	5.8873(7)	404.115(9)	2.01
375.03	8.2867(8)	5.8864(1)	404.224(1)	2.03
376.95	8.2888(1)	5.8853(8)	404.351(9)	2.06
378.86	8.2908(6)	5.8843(0)	404.476(7)	2.07
380.79	8.2928(5)	5.8831(1)	404.589(8)	2.07
382.55	8.2944(3)	5.8820(7)	404.672(1)	2.03
384.50	8.2959(3)	5.8809(7)	404.742(4)	1.99
386.28	8.2972(6)	5.8801(3)	404.814(6)	1.96
388.21	8.2984(5)	5.8794(2)	404.882(3)	1.92
390.08	8.2995(1)	5.8788(5)	404.946(3)	1.91
391.97	8.3004(8)	5.8784(3)	405.011(5)	1.94
393.74	8.3013(8)	5.8780(8)	405.075(1)	1.97
395.58	8.3021(7)	5.8778(5)	405.136(4)	2.01

Table S4. Evolution of refined lattice parameters in $Cs_{0.75}MA_{0.25}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
311.08	8.2728(5)	5.8932(0)	403.330(2)	1.76
313.07	8.2732(1)	5.8925(2)	403.319(1)	1.76
315.25	8.2742(5)	5.8922(4)	403.401(6)	1.72
317.25	8.2752(3)	5.8918(1)	403.467(8)	1.77
319.32	8.2763(5)	5.8914(3)	403.550(8)	1.76
321.06	8.2774(5)	5.8910(1)	403.629(6)	1.82
322.94	8.2782(7)	5.8904(6)	403.671(2)	1.83
324.89	8.2795(8)	5.8899(2)	403.762(8)	1.88
326.88	8.2810(0)	5.8893(0)	403.858(6)	1.89
328.70	8.2823(3)	5.8885(6)	403.937(2)	1.95
330.66	8.2840(6)	5.8877(3)	404.048(8)	1.97
332.60	8.2860(5)	5.8866(1)	404.166(2)	2.00
334.56	8.2883(3)	5.8853(3)	404.301(3)	2.10
336.39	8.2909(2)	5.8836(9)	404.441(2)	2.20
338.18	8.2934(2)	5.8820(0)	404.568(3)	2.24
340.25	8.2959(7)	5.8801(3)	404.688(9)	2.27
342.03	8.2982(7)	5.8784(9)	404.793(6)	2.21
343.89	8.3004(9)	5.8770(1)	404.915(0)	2.14
345.95	8.3026(9)	5.8753(4)	405.014(2)	2.08
347.77	8.3050(2)	5.8735(6)	405.118(7)	2.07
349.75	8.3060(9)	5.8735(0)	405.218(8)	2.14
351.63	8.3065(7)	5.8736(2)	405.275(2)	2.19
353.57	8.3071(7)	5.8739(6)	405.356(4)	2.23
355.50	8.3074(9)	5.8744(5)	405.421(6)	2.30
357.39	8.3082(7)	5.8747(6)	405.519(2)	2.26
359.36	8.3085(5)	5.8752(4)	405.579(5)	2.30

Table S5. Evolution of refined lattice parameters in $Cs_{0.63}MA_{0.37}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
257.80	8.2643(5)	5.8902(7)	402.302(2)	1.48
259.79	8.2654(0)	5.8902(6)	402.403(6)	1.54
261.73	8.2664(2)	5.8902(6)	402.502(4)	1.53
263.56	8.2673(7)	5.8901(5)	402.588(7)	1.52
265.44	8.2684(5)	5.8900(6)	402.687(8)	1.51
267.27	8.2695(9)	5.8898(4)	402.783(2)	1.54
269.05	8.2706(4)	5.8896(2)	402.870(8)	1.53
271.00	8.2718(5)	5.8894(1)	402.973(7)	1.55
272.89	8.2732(1)	5.8891(0)	403.085(0)	1.52
274.84	8.2744(9)	5.8887(2)	403.184(3)	1.54
276.75	8.2757(8)	5.8883(2)	403.282(6)	1.54
278.61	8.2771(9)	5.8878(6)	403.388(4)	1.53
280.53	8.2787(0)	5.8872(9)	403.496(3)	1.55
282.50	8.2802(4)	5.8866(6)	403.603(6)	1.53
284.36	8.2818(7)	5.8859(5)	403.713(9)	1.54
286.28	8.2836(2)	5.8852(2)	403.833(9)	1.57
288.21	8.2856(7)	5.8843(2)	403.972(2)	1.58
290.22	8.2880(1)	5.8831(0)	404.116(7)	1.61
292.01	8.2909(4)	5.8813(6)	404.282(6)	1.66
293.79	8.2953(2)	5.8785(5)	404.516(5)	1.68
295.80	8.2991(5)	5.8756(0)	404.686(7)	1.71
297.70	8.3025(2)	5.8726(5)	404.812(0)	1.71
299.63	8.3038(5)	5.8721(1)	404.905(1)	1.72
301.54	8.3046(0)	5.8726(6)	405.016(2)	1.81
303.30	8.3052(6)	5.8732(3)	405.119(4)	1.86
305.25	8.3058(1)	5.8732(6)	405.175(2)	1.91
307.09	8.3065(6)	5.8738(2)	405.287(1)	1.94
309.03	8.3071(3)	5.8743(9)	405.381(9)	2.00

Table S6. Evolution of refined lattice parameters in $Cs_{0.5}MA_{0.5}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
234.05	8.2748(8)	5.8879(8)	403.171(4)	1.60
236.02	8.2759(7)	5.8876(9)	403.257(5)	1.62
238.03	8.2771(1)	5.8872(8)	403.340(6)	1.61
240.06	8.2785(2)	5.8867(8)	403.443(9)	1.58
242.09	8.2799(7)	5.8863(2)	403.553(9)	1.54
244.08	8.2814(9)	5.8858(0)	403.666(5)	1.53
245.90	8.2830(5)	5.8852(0)	403.777(0)	1.51
247.81	8.2846(8)	5.8844(6)	403.884(7)	1.50
249.69	8.2866(0)	5.8837(0)	404.020(9)	1.51
251.61	8.2887(5)	5.8827(6)	404.164(8)	1.52
253.50	8.2912(2)	5.8816(0)	404.326(8)	1.53
255.38	8.2945(9)	5.8800(0)	404.545(9)	1.58
257.19	8.2982(8)	5.8777(6)	404.751(4)	1.63
258.92	8.3017(7)	5.8749(1)	404.895(0)	1.69
260.91	8.3047(4)	5.8727(8)	405.038(2)	1.80
262.90	8.3054(9)	5.8731(5)	405.136(5)	1.97
264.70	8.3059(2)	5.8736(7)	405.214(8)	2.07
266.56	8.3064(4)	5.8738(6)	405.278(4)	2.15
268.62	8.3074(1)	5.8742(6)	405.400(1)	2.22
270.52	8.3077(5)	5.8746(9)	405.463(0)	2.26
272.45	8.3084(1)	5.8753(4)	405.573(3)	2.32
274.35	8.3089(5)	5.8755(1)	405.637(1)	2.31
276.20	8.3097(5)	5.8761(1)	405.756(8)	2.33
278.20	8.3106(6)	5.8762(4)	405.854(4)	2.32
280.15	8.3109(3)	5.8769(0)	405.927(3)	2.41
282.00	8.3115(5)	5.8775(0)	406.029(2)	2.38
283.48	8.3120(4)	5.8776(6)	406.087(6)	2.39
283.46	8.3124(8)	5.8781(0)	406.160(8)	2.35
283.20	8.3125(3)	5.8780(8)	406.164(8)	2.36
283.12	8.3126(1)	5.8781(3)	406.176(4)	2.38
283.04	8.3126(7)	5.8781(7)	406.184(8)	2.37
282.97	8.3128(5)	5.8782(7)	406.208(9)	2.36

Table S7. Evolution of refined lattice parameters in $Cs_{0.37}MA_{0.63}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
198.11	8.2804(4)	5.8830(1)	403.372(6)	1.81
200.09	8.2814(8)	5.8827(8)	403.458(1)	1.79
202.25	8.2827(7)	5.8823(8)	403.556(3)	1.79
204.18	8.2840(7)	5.8820(5)	403.661(1)	1.81
206.17	8.2854(7)	5.8816(7)	403.771(2)	1.77
207.99	8.2868(7)	5.8812(6)	403.879(2)	1.78
209.87	8.2883(8)	5.8808(3)	403.996(7)	1.81
211.80	8.2898(4)	5.8803(2)	404.104(5)	1.82
213.59	8.2915(7)	5.8796(6)	404.227(1)	1.81
215.38	8.2935(2)	5.8789(3)	404.366(9)	1.81
217.37	8.2959(8)	5.8777(2)	404.523(5)	1.80
219.38	8.2995(1)	5.8755(1)	404.716(1)	1.81
221.08	8.3034(2)	5.8722(5)	404.872(8)	1.90
222.90	8.3043(7)	5.8727(7)	405.001(2)	2.03
224.83	8.3052(0)	5.8728(4)	405.086(8)	2.11
226.69	8.3060(8)	5.8733(6)	405.208(6)	2.17
228.52	8.3068(1)	5.8737(3)	405.305(8)	2.21
230.30	8.3073(3)	5.8742(9)	405.394(3)	2.23
232.19	8.3081(1)	5.8749(4)	405.516(0)	2.23
234.00	8.3087(6)	5.8757(4)	405.634(8)	2.20
235.78	8.3095(0)	5.8757(5)	405.707(4)	2.25
237.72	8.3102(8)	5.8763(1)	405.822(6)	2.20
239.61	8.3109(0)	5.8767(0)	405.909(9)	2.23
241.41	8.3115(8)	5.8772(1)	406.011(6)	2.21
243.30	8.3122(7)	5.8778(6)	406.124(4)	2.23
245.20	8.3130(9)	5.8785(8)	406.253(9)	2.22
247.23	8.3137(1)	5.8791(7)	406.355(1)	2.22

Table S8. Evolution of refined lattice parameters in $Cs_{0.25}MA_{0.75}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
176.04	8.2987(0)	5.8759(2)	404.665(4)	1.09
177.97	8.2995(5)	5.8761(5)	404.764(0)	1.07
180.10	8.3005(4)	5.8762(7)	404.869(0)	1.11
182.09	8.3015(7)	5.8765(8)	404.990(7)	1.08
184.08	8.3025(7)	5.8766(2)	405.090(9)	1.08
185.89	8.3037(7)	5.8770(8)	405.239(7)	1.08
187.80	8.3047(6)	5.8770(9)	405.336(6)	1.10
189.67	8.3059(8)	5.8772(1)	405.464(5)	1.14
191.58	8.3068(3)	5.8776(9)	405.580(8)	1.13
193.39	8.3080(3)	5.8775(4)	405.687(4)	1.15
195.15	8.3092(0)	5.8777(6)	405.816(3)	1.14
197.08	8.3102(3)	5.8780(3)	405.935(7)	1.14
198.90	8.3111(9)	5.8785(3)	406.064(0)	1.17
200.78	8.3117(5)	5.8791(0)	406.159(1)	1.16
202.60	8.3128(2)	5.8794(4)	406.287(1)	1.17
204.37	8.3136(4)	5.8798(8)	406.396(9)	1.20
206.32	8.3145(1)	5.8803(4)	406.514(6)	1.18
208.23	8.3155(1)	5.8807(6)	406.640(4)	1.23
210.12	8.3162(9)	5.8812(0)	406.747(7)	1.21
212.03	8.3170(5)	5.8818(6)	406.867(3)	1.23
213.97	8.3175(9)	5.8827(3)	406.980(9)	1.23
215.82	8.3186(3)	5.8829(4)	407.097(2)	1.21
217.73	8.3190(8)	5.8838(4)	407.203(5)	1.20
219.62	8.3202(1)	5.8839(2)	407.319(5)	1.23
221.51	8.3207(6)	5.8847(4)	407.429(7)	1.20
223.39	8.3217(7)	5.8849(0)	407.540(9)	1.21
225.23	8.3221(1)	5.8858(0)	407.635(4)	1.24

Table S9. Evolution of refined lattice parameters in $Cs_{0.13}MA_{0.87}PbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
151.03	5.8774(9)		203.036(7)	2.54
152.85	5.8779(2)		203.081(3)	2.55
155.05	5.8784(1)		203.133(0)	2.51
157.16	5.8790(3)		203.197(0)	2.50
159.07	5.8795(8)		203.253(8)	2.50
161.01	5.8800(6)		203.303(6)	2.56

Table S10. Evolution of refined lattice parameters in $MAPbBr_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
169.80	8.3306(4)	5.9545(7)	413.244(7)	3.44
171.16	8.3308(4)	5.9544(8)	413.257(4)	3.46
172.46	8.3313(3)	5.9544(4)	413.303(8)	3.67
173.75	8.3318(4)	5.9542(3)	413.340(1)	3.50
175.19	8.3324(6)	5.9540(1)	413.385(8)	3.47
176.60	8.3331(7)	5.9538(5)	413.445(8)	3.48
177.77	8.3339(2)	5.9538(0)	413.516(2)	3.43
180.09	8.3346(0)	5.9536(0)	413.569(6)	3.29
181.37	8.3356(1)	5.9531(5)	413.639(5)	3.22
182.56	8.3361(2)	5.9532(4)	413.695(5)	3.65
183.77	8.3369(1)	5.9530(7)	413.762(4)	3.68
185.20	8.3376(2)	5.9527(3)	413.809(9)	3.57
186.38	8.3382(7)	5.9526(0)	413.864(2)	3.58
187.68	8.3389(5)	5.9523(0)	413.911(6)	3.60
189.09	8.3395(9)	5.9519(7)	413.951(8)	3.91
190.98	8.3405(3)	5.9515(4)	414.016(1)	3.67
192.36	8.3414(4)	5.9512(3)	414.084(4)	3.56
193.88	8.3423(3)	5.9508(4)	414.145(7)	3.71
196.57	8.3432(3)	5.9503(6)	414.201(1)	3.56
198.07	8.3446(2)	5.9497(0)	414.293(4)	3.65
199.40	8.3457(2)	5.9493(7)	414.379(8)	3.67
200.79	8.3465(7)	5.9489(4)	414.434(3)	3.84
202.08	8.3474(9)	5.9486(0)	414.501(7)	3.98
203.29	8.3482(4)	5.9481(9)	414.548(1)	3.85
205.06	8.3492(4)	5.9477(3)	414.615(4)	3.85
206.48	8.3500(3)	5.9468(0)	414.628(8)	3.89
207.81	8.3512(8)	5.9463(2)	414.719(8)	3.81
210.87	8.3526(6)	5.9458(1)	414.820(9)	3.71
212.68	8.3547(9)	5.9447(6)	414.959(9)	3.83
214.03	8.3560(3)	5.9441(0)	415.036(1)	3.66
215.43	8.3569(2)	5.9433(7)	415.073(5	3.74
216.63	8.3580(1)	5.9428(2)	415.144(1)	3.75
217.91	8.3590(5)	5.9422(4)	415.206(7)	3.82
219.44	8.3601(6)	5.9415(6)	415.268(9)	3.85
220.92	8.3613(6)	5.9408(0)	415.334(7)	3.79
222.29	8.3626(9)	5.9398(0)	415.397(2)	3.59
224.06	8.3640(1)	5.9389(4)	415.468(3)	3.43
225.69	8.3654(3)	5.9377(3)	415.525(4)	3.17
229.20	8.3679(3)	5.9359(5)	415.647(8)	3.04
231.34	8.3705(8)	5.9332(6)	415.724(1)	2.66
232.90	8.3728(7)	5.9311(9)	415.805(4)	2.39
234.70	8.3751(1)	5.9291(1)	415.881(7)	2.53
236.18	8.3778(1)	5.9268(4)	415.991(5)	2.65
237.49	8.3798(1)	5.9254(9)	416.094(9)	2.60

238.92	8.3801(2)	5.9258(0)	416.147(9)	2.94
240.27	8.3804(1)	5.9261(0)	416.197(7)	2.97
242.38	8.3810(6)	5.9265(3)	416.292(2)	2.90
243.84	8.3816(8)	5.9269(6)	416.384(4)	3.04
245.23	8.3822(9)	5.9271(2)	416.456(3)	3.00
246.36	8.3825(7)	5.9276(8)	416.522(7)	3.11
248.10	8.3831(0)	5.9279(4)	416.593(8)	3.00
249.57	8.3837(5)	5.9282(5)	416.681(0)	3.05
250.99	8.3840(6)	5.9287(1)	416.743(1)	3.01
252.37	8.3845(3)	5.9289(6)	416.808(0)	3.06
253.77	8.3850(9)	5.9293(9)	416.894(0)	2.89
255.20	8.3854(5)	5.9296(6)	416.948(7)	3.02
256.70	8.3859(6)	5.9299(6)	417.020(9)	3.17
258.08	8.3864(5)	5.9303(4)	417.095(8)	2.92
259.50	8.3871(7)	5.9305(2)	417.179(6)	2.84
262.63	8.3874(1)	5.9311(1)	417.245(2)	3.00
265.18	8.3887(5)	5.9318(0)	417.427(5)	2.96
268.10	8.3897(1)	5.9323(8)	417.563(2)	3.04
273.47	8.3913(9)	5.9335(3)	417.812(0)	2.91
274.79	8.3926(7)	5.9345(0)	418.007(5)	3.19
277.17	8.3930(7)	5.9349(6)	418.080(2)	3.27
280.21	8.3940(0)	5.9355(9)	418.217(5)	3.07
281.60	8.3950(2)	5.9362(6)	418.366(3)	3.43
283.13	8.3955(7)	5.9365(8)	418.443(2)	3.35
284.51	8.3959(6)	5.9369(2)	418.505(6)	3.41
285.79	8.3965(3)	5.9372(5)	418.585(8)	3.40
287.09	8.3969(3)	5.9376(1)	418.651(6)	3.43
288.61	8.3973(3)	5.9378(5)	418.708(6)	3.49
290.27	8.3976(9)	5.9382(2)	418.770(3)	3.59
292.56	8.3985(9)	5.9385(9)	418.886(4)	3.54
295.56	8.3993(4)	5.9390(3)	418.992(4)	3.55
296.83	8.4001(0)	5.9397(1)	419.115(7)	3.71
297.93	8.4003(9)	5.9400(4)	419.168(8)	3.66
299.32	8.4007(7)	5.9402(8)	419.223(1)	3.73
300.58	8.4012(1)	5.9405(9)	419.288(9)	3.58
301.69	8.4017(3)	5.9407(9)	419.354(5)	3.58
301.73	8.4018(1)	5.9409(2)	419.372(7)	3.53

Table S11. Evolution of refined lattice parameters in $CsPbCl_3$.

Temperature (K)	*a* (Å)	*b* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
290	7.895(7)	11.232(0)	7.894(4)	700.12(4)	5.94
295	7.898(1)	11.235(9)	7.897(3)	700.83(8)	4.70
300	7.900(1)	11.238(6)	7.899(7)	701.39(5)	4.13
305	7.902(3)	11.240(9)	7.902(1)	701.95(1)	3.64
310	7.904(5)	11.242(9)	7.904(4)	702.47(0)	3.22
315	7.906(8)		5.622(1)	351.48(9)	2.99
320	7.909(6)		5.622(0)	351.73(6)	2.71
325	7.913(8)		5.619(5)	351.96(7)	2.43
330	7.916(3)		5.618(9)	352.15(5)	2.38
335	7.918(5)		5.619(1)	352.35(7)	2.17
340	7.920(0)		5.619(3)	352.51(3)	2.11
345	7.921(7)		5.619(8)	352.68(9)	1.88
350	7.923(2)		5.620(3)	352.85(9)	1.77
355	7.924(5)		5.620(8)	353.01(1)	1.67
360	7.926(0)		5.621(2)	353.16(9)	1.57

Table S12. Evolution of refined lattice parameters in $Cs_{0.87}MA_{0.13}PbCl_3$.

Temperature (K)	*a* (Å)	*b* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
100	7.870(6)	11.179(8)	7.784(0)	684.94(0)	0.07
105	7.871(1)	11.180(1)	7.784(9)	685.07(9)	0.11
110	7.870(8)	11.179(5)	7.788(1)	685.29(8)	0.04
115	7.870(8)	11.179(9)	7.791(8)	685.64(6)	0.03
120	7.870(3)	11.180(2)	7.793(4)	685.76(6)	0.08
125	7.869(6)	11.180(4)	7.797(2)	686.04(8)	0.08
130	7.869(1)	11.180(9)	7.798(9)	686.17(9)	0.07
135	7.869(5)	11.180(6)	7.802(6)	686.53(1)	0.05
140	7.868(5)	11.181(7)	7.805(7)	686.78(0)	0.04
145	7.868(7)	11.183(7)	7.805(6)	686.91(0)	0.13
150	7.868(1)	11.183(7)	7.806(6)	686.94(7)	0.09
155	7.869(1)	11.185(1)	7.809(0)	687.32(8)	0.11
160	7.868(8)	11.186(0)	7.811(6)	687.59(2)	0.03
165	7.867(7)	11.186(7)	7.814(9)	687.82(9)	0.03
170	7.868(2)	11.188(7)	7.816(8)	688.16(1)	0.09
175	7.868(9)	11.188(5)	7.819(3)	688.42(8)	0.08
180	7.869(9)	11.188(7)	7.822(9)	688.84(3)	0.04
185	7.869(8)	11.189(9)	7.827(0)	689.27(6)	0.07
190	7.870(5)	11.190(2)	7.830(0)	689.62(3)	0.04
195	7.871(9)	11.191(2)	7.832(4)	690.01(6)	0.04
200	7.872(5)	11.192(0)	7.834(6)	690.30(4)	0.09
205	7.873(8)	11.192(4)	7.837(5)	690.70(1)	0.09
210	7.875(1)	11.192(1)	7.841(3)	691.13(2)	0.03
215	7.876(4)	11.193(2)	7.844(2)	691.57(4)	0.03
220	7.878(0)	11.195(3)	7.846(0)	692.00(3)	0.03
225	7.873(8)		5.598(6)	347.09(5)	0.65
230	7.876(0)		5.599(9)	347.37(4)	0.62
235	7.878(7)		5.600(2)	347.63(3)	0.66
240	7.880(9)		5.601(4)	347.90(4)	0.62
245	7.883(2)		5.602(5)	348.17(0)	0.67
250	7.885(7)		5.603(5)	348.45(7)	0.68
255	7.887(7)		5.604(4)	348.69(3)	0.57
260	7.889(7)		5.605(7)	348.95(3)	0.63
265	7.891(3)		5.606(5)	349.13(8)	0.64
270	7.894(1)		5.607(6)	349.45(9)	0.67
275	7.897(3)		5.609(3)	349.84(2)	0.69
280	7.900(8)		5.610(4)	350.21(6)	0.76
285	7.903(4)		5.611(8)	350.53(6)	0.74
290	7.905(8)		5.612(7)	350.81(3)	0.75
295	7.907(9)		5.613(8)	351.06(2)	0.72
300	7.909(5)		5.614(7)	351.26(5)	0.74
305	7.911(1)		5.615(9)	351.48(1)	0.70
310	7.913(0)		5.617(0)	351.72(3)	0.67
315	7.914(9)		5.618(4)	351.97(4)	0.69

320	7.916(5)	5.619(6)	352.19(2)	0.74
325	7.918(1)	5.620(9)	352.40(9)	0.68
330	7.919(7)	5.622(1)	352.63(9)	0.64
335	7.921(2)	5.623(4)	352.85(3)	0.67
340	7.923(1)	5.625(1)	353.12(0)	0.63

Table S13. Evolution of refined lattice parameters in $Cs_{0.75}MA_{0.25}PbCl_3$.

Temperature (K)	*a* (Å)	*b* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
100	7.900(9)	11.188(5)	7.809(4)	690.35(5)	1.37
105	7.900(0)	11.189(7)	7.810(0)	690.40(3)	1.36
110	7.899(8)	11.190(2)	7.811(3)	690.54(0)	1.41
115	7.899(0)	11.190(0)	7.813(2)	690.62(1)	1.39
120	7.898(4)	11.190(8)	7.815(0)	690.76(9)	1.40
125	7.898(1)	11.191(3)	7.818(2)	691.06(2)	1.41
130	7.897(7)	11.191(3)	7.820(0)	691.18(1)	1.42
135	7.896(8)	11.191(0)	7.823(6)	691.41(1)	1.38
140	7.896(8)	11.191(6)	7.826(4)	691.68(3)	1.44
145	7.896(2)	11.191(7)	7.829(6)	691.92(8)	1.42
150	7.894(6)	11.190(0)	7.835(2)	692.17(2)	1.41
155	7.894(0)	11.189(7)	7.840(0)	692.53(2)	1.41
160	7.894(2)	11.189(6)	7.843(9)	692.87(8)	1.47
165	7.894(2)	11.189(3)	7.847(5)	693.18(6)	1.48
170	7.894(8)	11.189(3)	7.850(9)	693.53(9)	1.51
175	7.895(4)	11.190(1)	7.853(6)	693.87(6)	1.52
180	7.896(2)	11.190(1)	7.857(6)	694.30(9)	1.56
185	7.897(1)	11.190(5)	7.860(0)	694.61(9)	1.59
190	7.898(5)	11.191(3)	7.862(8)	695.03(6)	1.65
195	7.899(8)	11.192(6)	7.865(0)	695.43(0)	1.64
200	7.901(9)	11.194(0)	7.867(5)	695.93(1)	1.68
205	7.889(1)		5.597(2)	348.36(6)	2.01
210	7.891(1)		5.597(9)	348.58(5)	2.07
215	7.893(1)		5.598(5)	348.79(9)	2.06
220	7.894(8)		5.599(5)	349.01(3)	2.08
225	7.896(6)		5.600(6)	349.23(7)	2.12
230	7.898(3)		5.601(7)	349.46(0)	2.15
235	7.900(2)		5.602(8)	349.69(5)	2.13
240	7.902(2)		5.603(8)	349.93(5)	2.22
245	7.904(0)		5.604(9)	350.16(3)	2.19
250	7.905(6)		5.605(7)	350.35(8)	2.22
255	7.906(9)		5.606(6)	350.53(2)	2.22
260	7.908(5)		5.607(6)	350.72(8)	2.22
265	7.909(7)		5.608(4)	350.88(3)	2.20
270	7.911(0)		5.609(2)	351.05(6)	2.21
275	7.912(3)		5.610(1)	351.22(2)	2.21
280	7.913(8)		5.611(1)	351.42(2)	2.22
285	7.915(0)		5.611(9)	351.57(6)	2.24
290	7.916(4)		5.612(8)	351.75(5)	2.20
295	7.917(3)		5.613(6)	351.88(9)	2.22
300	7.918(8)		5.614(5)	352.07(7)	2.22
305	7.919(9)		5.615(4)	352.22(7)	2.18
310	7.920(6)		5.616(1)	352.33(2)	2.21

Table S14. Evolution of refined lattice parameters in $Cs_{0.63}MA_{0.37}PbCl_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
100	7.887(1)	5.632(8)	350.40(7)	3.03
110	7.888(8)	5.632(4)	350.52(7)	2.99
120	7.889(9)	5.629(6)	350.45(1)	2.93
130	7.892(8)	5.627(9)	350.60(6)	2.91
140	7.896(3)	5.627(3)	350.87(6)	2.93
150	7.899(2)	5.624(6)	350.96(8)	2.91
155	7.901(8)	5.625(0)	351.21(9)	2.94
160	7.903(3)	5.623(1)	351.24(3)	2.95
165	7.906(4)	5.623(5)	351.53(6)	2.94
170	7.908(2)	5.621(8)	351.59(2)	2.97
175	7.910(4)	5.621(5)	351.76(4)	2.99
180	7.913(9)	5.622(2)	352.12(1)	2.96
185	7.915(7)	5.620(6)	352.18(2)	3.01
190	7.919(2)	5.621(3)	352.54(2)	3.00
195	7.921(5)	5.620(3)	352.67(8)	3.01
200	7.924(4)	5.620(8)	352.96(5)	2.98
205	7.928(1)	5.620(3)	353.27(3)	2.79
210	7.931(8)	5.620(8)	353.62(6)	2.52
215	7.934(4)	5.622(3)	353.95(5)	2.51
220	7.935(1)	5.622(3)	354.02(6)	2.52
225	7.937(4)	5.623(9)	354.32(4)	2.54
230	7.937(5)	5.623(9)	354.33(7)	2.69
240	7.940(8)	5.626(3)	354.78(1)	2.73
250	7.943(7)	5.627(8)	355.12(7)	2.70
260	7.947(1)	5.630(0)	355.58(4)	2.56
270	7.951(1)	5.632(5)	356.09(4)	2.40
280	7.953(9)	5.634(6)	356.47(3)	2.39
290	7.955(2)	5.636(6)	356.72(0)	2.45

Table S15. Evolution of refined lattice parameters in $Cs_{0.5}MA_{0.5}PbCl_3$.

Temperature (K)	a (Å)	c (Å)	Cell volume (Å3)	R_{Bragg}
100	7.896(0)	5.607(8)	349.62(8)	2.93
105	7.896(5)	5.608(4)	349.71(8)	3.00
110	7.897(4)	5.609(2)	349.84(2)	2.97
115	7.898(2)	5.610(0)	349.96(5)	2.94
120	7.899(4)	5.611(0)	350.13(8)	3.02
125	7.900(4)	5.611(7)	350.26(5)	3.01
130	7.901(8)	5.612(9)	350.46(8)	2.99
135	7.903(2)	5.614(0)	350.66(4)	3.00
140	7.904(6)	5.615(0)	350.85(1)	2.96
145	7.906(4)	5.616(7)	351.11(5)	2.96
150	7.908(0)	5.617(6)	351.31(1)	3.05
155	7.909(7)	5.618(7)	351.53(1)	2.96
160	7.911(2)	5.619(9)	351.74(1)	3.12
165	7.912(9)	5.620(9)	351.95(1)	3.07
170	7.914(7)	5.621(8)	352.16(7)	3.16
175	7.916(3)	5.623(0)	352.38(2)	3.15
180	7.917(8)	5.623(8)	352.57(0)	3.08
185	7.919(6)	5.624(9)	352.80(1)	3.25
190	7.921(1)	5.625(9)	352.99(9)	3.23
195	7.922(8)	5.627(2)	353.23(2)	3.30
200	7.924(7)	5.628(4)	353.47(5)	3.18
205	7.926(3)	5.629(6)	353.69(1)	3.30
210	7.928(2)	5.630(8)	353.93(2)	3.23
215	7.929(9)	5.632(2)	354.17(3)	3.28
220	7.931(3)	5.633(3)	354.37(1)	3.29
225	7.932(6)	5.634(5)	354.56(9)	3.22
230	7.934(2)	5.635(6)	354.77(6)	3.28
235	7.935(8)	5.637(0)	355.01(0)	3.35
240	7.937(1)	5.638(0)	355.18(7)	3.33
245	7.938(5)	5.639(2)	355.38(8)	3.37
250	7.940(2)	5.640(4)	355.61(9)	3.39
255	7.941(8)	5.641(5)	355.82(7)	3.45
260	7.943(4)	5.642(6)	356.04(1)	3.40
265	7.945(0)	5.643(8)	356.25(6)	3.58
270	7.946(6)	5.644(7)	356.46(6)	3.48
275	7.948(1)	5.645(8)	356.66(6)	3.65
280	7.949(6)	5.646(9)	356.87(2)	3.65
285	7.951(2)	5.648(0)	357.07(9)	3.77
290	7.952(4)	5.648(5)	357.22(0)	3.63

Table S16. Evolution of refined lattice parameters in $Cs_{0.37}MA_{0.63}PbCl_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
100	7.948(2)	5.626(6)	355.45(9)	4.01
105	7.949(8)	5.626(8)	355.61(9)	4.01
110	7.950(2)	5.626(9)	355.65(5)	3.95
115	7.952(2)	5.627(6)	355.88(0)	4.32
120	7.954(0)	5.628(2)	356.08(3)	4.25
125	7.955(5)	5.628(8)	356.25(3)	4.24
130	7.956(9)	5.629(4)	356.42(3)	4.14
135	7.958(2)	5.629(9)	356.57(0)	4.17
140	7.960(2)	5.630(8)	356.79(6)	4.18
145	7.961(8)	5.631(8)	357.00(8)	4.06
150	7.962(7)	5.632(3)	357.11(6)	4.23
155	7.965(0)	5.633(5)	357.39(9)	4.25
160	7.966(9)	5.634(9)	357.66(0)	4.25
165	7.968(6)	5.635(8)	357.87(6)	4.28
170	7.970(6)	5.636(9)	358.12(1)	4.28
175	7.972(2)	5.638(0)	358.33(9)	4.29
180	7.974(2)	5.639(1)	358.58(8)	4.32
185	7.976(1)	5.640(2)	358.82(3)	4.23
190	7.977(8)	5.641(3)	359.04(6)	4.40
195	7.979(7)	5.642(3)	359.28(0)	4.57
200	7.981(1)	5.643(2)	359.46(6)	4.53
205	7.982(8)	5.644(3)	359.69(3)	4.66
210	7.984(4)	5.645(4)	359.90(4)	4.73
215	7.986(0)	5.646(6)	360.12(4)	4.67
220	7.987(8)	5.647(5)	360.34(6)	4.77
225	7.989(3)	5.649(1)	360.58(1)	4.76
230	7.991(3)	5.649(9)	360.81(3)	5.09
235	7.993(6)	5.651(4)	361.11(6)	5.14
240	7.995(9)	5.652(7)	361.41(1)	4.88
245	7.997(5)	5.653(5)	361.61(1)	4.94
250	7.999(2)	5.654(4)	361.81(3)	5.02
255	8.000(4)	5.655(0)	361.96(5)	5.10
260	8.002(1)	5.655(9)	362.17(4	5.20
265	8.004(1)	5.657(1)	362.43(0)	5.20
270	8.005(7)	5.658(2)	362.64(4)	5.23
275	8.007(6)	5.659(2)	362.88(3)	5.62
280	8.008(9)	5.659(8)	363.04(0)	5.59
285	8.010(7)	5.660(7)	363.25(9)	5.66
290	8.012(1)	5.661(3)	363.42(1)	5.43

Table S17. Evolution of refined lattice parameters in $Cs_{0.25}MA_{0.75}PbCl_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
100	7.943(1)	5.626(0)	354.96(2)	2.20
105	7.944(0)	5.626(3)	355.06(8)	2.20
110	7.944(6)	5.627(2)	355.17(3)	2.24
115	7.945(2)	5.627(7)	355.26(3)	2.23
120	7.946(2)	5.628(5)	355.40(6)	2.22
125	7.947(0)	5.629(2)	355.51(6)	2.23
130	7.948(4)	5.630(2)	355.70(0)	2.21
135	7.949(5)	5.630(7)	355.83(3)	2.18
140	7.950(8)	5.631(5)	356.00(4)	2.21
145	7.952(6)	5.632(2)	356.20(7)	2.16
150	7.953(6)	5.633(3)	356.37(0)	2.19
155	7.955(3)	5.634(1)	356.56(4)	2.15
160	7.956(6)	5.635(1)	356.75(3)	2.17
165	7.958(3)	5.636(1)	356.96(2)	2.18
170	7.959(9)	5.637(1)	357.17(9)	2.17
175	7.961(6)	5.638(2)	357.40(0)	2.14
180	7.963(5)	5.639(4)	357.64(4)	2.13
185	7.965(1)	5.640(6)	357.86(3)	2.19
190	7.967(1)	5.641(7)	358.11(4)	2.15
195	7.968(7)	5.642(7)	358.31(8)	2.16
200	7.970(4)	5.643(7)	358.53(9)	2.18
205	7.972(3)	5.645(0)	358.78(8)	2.20
210	7.973(9)	5.646(0)	358.99(7)	2.21
215	7.975(8)	5.647(2)	359.24(4)	2.25
220	7.977(7)	5.648(1)	359.46(8)	2.25
225	7.979(4)	5.649(1)	359.68(8)	2.26
230	7.981(2)	5.650(1)	359.91(0)	2.31
235	7.983(1)	5.651(0)	360.14(2)	2.31
240	7.984(8)	5.651(7)	360.34(6)	2.32
245	7.986(5)	5.652(6)	360.55(4)	2.36
250	7.988(4)	5.653(5)	360.77(9)	2.41
255	7.990(4)	5.654(2)	361.00(5)	2.44
260	7.991(9)	5.654(8)	361.18(4)	2.41
265	7.993(7)	5.655(7)	361.40(8)	2.48
270	7.995(6)	5.656(5)	361.62(7)	2.47
275	7.997(2)	5.657(2)	361.81(3)	2.50
280	7.998(8)	5.657(8)	362.00(1)	2.52
285	8.000(9)	5.658(4)	362.22(6)	2.60
290	8.002(6)	5.659(1)	362.42(5)	2.53

Table S18. Evolution of refined lattice parameters in $Cs_{0.13}MA_{0.87}PbCl_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
100	7.959(4)	5.649(0)	357.88(1)	4.95
105	7.959(1)	5.650(3)	357.94(0)	4.91
110	7.959(7)	5.651(3)	358.05(3)	4.88
115	7.960(4)	5.652(2)	358.17(7)	4.88
120	7.961(0)	5.652(8)	358.26(8)	4.86
125	7.962(1)	5.653(9)	358.43(5)	4.82
130	7.962(8)	5.654(6)	358.54(4)	4.80
135	7.963(7)	5.655(4)	358.67(1)	4.77
140	7.965(0)	5.656(3)	358.85(4)	4.78
145	7.965(8)	5.656(8)	358.95(7)	4.76
150	7.966(9)	5.657(3)	359.08(4)	4.71
155	7.968(0)	5.657(6)	359.20(4)	4.66
160	7.968(9)	5.657(7)	359.28(7)	4.64
165	7.970(0)	5.658(2)	359.42(0)	4.62
170	7.971(7)	5.659(2)	359.63(4)	4.60
175	7.973(4)	5.660(2)	359.85(3)	4.61
180	7.975(3)	5.661(4)	360.09(9)	4.61
185	7.977(2)	5.662(4)	360.33(5)	4.59
190	7.979(1)	5.663(5)	360.58(3)	4.58
195	7.981(0)	5.664(7)	360.82(5)	4.53
200	7.982(8)	5.665(7)	361.05(8)	4.51
205	7.984(7)	5.666(7)	361.28(9)	4.43
210	7.986(5)	5.667(8)	361.52(5)	4.16
215	7.988(3)	5.669(1)	361.76(2)	3.72
220	7.989(8)	5.670(1)	361.97(0)	3.71
225	7.991(5)	5.671(2)	362.18(7)	3.71
230	7.992(9)	5.672(2)	362.38(3)	3.71
235	7.994(5)	5.673(4)	362.60(3)	3.70
240	7.996(0)	5.674(3)	362.80(2)	3.69
245	7.997(6)	5.675(2)	363.00(5)	3.68
250	7.999(1)	5.676(2)	363.20(0)	3.66
255	8.000(5)	5.677(3)	363.40(3)	3.66
260	8.001(9)	5.678(2)	363.58(3)	3.66
265	8.003(4)	5.679(3)	363.79(0)	3.64
270	8.004(9)	5.680(1)	363.98(3)	3.62
275	8.006(4)	5.681(1)	364.17(5)	3.60
280	8.007(8)	5.681(9)	364.35(3)	3.56
285	8.009(2)	5.682(7)	364.53(1)	3.52
290	8.010(5)	5.683(2)	364.69(0)	3.51

Table S19. Evolution of refined lattice parameters in $MAPbCl_3$.

Temperature (K)	*a* (Å)	*c* (Å)	Cell volume (Å^3)	R_{Bragg}
165.67	8.0340(6)	5.6604(4)	365.359(4)	1.36
167.23	8.0339(3)	5.6604(5)	365.348(2)	1.36
168.50	8.0332(6)	5.6608(7)	365.314(4)	1.48
170.15	8.0328(1)	5.6610(8)	365.287(0)	1.33
171.79	8.0305(2)	5.6624(3)	365.165(8)	1.26
173.40	8.0235(1)	5.6649(5)	364.690(8)	1.28
174.80	8.0194(2)	5.6669(3)	364.446(4)	1.14
176.30	8.0178(7)	5.6678(0)	364.361(5)	1.36
178.95	8.0179(8)	5.6684(4)	364.412(6)	1.72
181.51	8.0183(6)	5.6689(0)	364.476(8)	1.92
185.61	8.0195(5)	5.6698(3)	364.644(8)	2.01
192.78	8.0215(9)	5.6711(0)	364.912(0)	2.34
196.68	8.0226(9)	5.6718(9)	365.063(0)	2.44
201.99	8.0239(5)	5.6728(3)	365.238(2)	2.55
207.13	8.0258(1)	5.6740(9)	365.488(7)	2.73
211.35	8.0269(3)	5.6748(9)	365.642(2)	2.87
215.10	8.0280(9)	5.6757(7)	365.804(6)	2.98
218.98	8.0291(8)	5.6765(9)	365.956(8)	3.14
223.43	8.0304(9)	5.6775(6)	366.138(8)	3.33
227.62	8.0316(4)	5.6784(2)	366.299(2)	3.47
231.47	8.0328(2)	5.6792(2)	366.458(4)	3.64
235.57	8.0339(6)	5.6800(3)	366.614(7)	3.84
239.35	8.0350(5)	5.6807(9)	366.763(3)	3.97
243.47	8.0362(3)	5.6815(5)	366.920(1)	4.13
247.68	8.0373(9)	5.6824(5)	367.084(2)	4.36
251.69	8.0385(8)	5.6833(0)	367.247(8)	4.51
255.67	8.0396(3)	5.6840(2)	367.390(3)	4.70
260.60	8.0407(6)	5.6847(8)	367.542(7)	4.88
265.11	8.0421(4)	5.6857(5)	367.731(6)	5.11
269.61	8.0433(4)	5.6866(0)	367.896(4)	5.36
273.79	8.0446(3)	5.6874(7)	368.070(7)	5.61
278.01	8.0458(3)	5.6883(1)	368.234(9)	5.58
282.20	8.0469(5)	5.6891(0)	368.388(5)	5.86
286.21	8.0480(1)	5.6898(6)	368.534(8)	5.93