Supplementary Information (SI) for Journal of Materials Chemistry C.

Supporting Information

Monoclinic crystal structure and a reusable stress-controlled optoelectronic switch in a lead halide perovskite, $CsPbBr_3$

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Table S1. Intensity statistics for XRD data for the superstructure of $CsPbBr_3$ ($P2_1/m$; V = 1590.5 Å^3).

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/σ	R(int)	Rσ
Inf - 2.25	173	177	97.7	5.51	40.2	10.8	0.0307	0.0605
2.25 - 1.75	178	179	99.4	6.35	26.6	10.92	0.0373	0.0567
1.75 - 1.52	172	177	97.2	6.17	17.4	10.29	0.0473	0.054
1.52 - 1.37	183	183	100	6.51	18.2	6.54	0.0402	0.0596
1.37 - 1.27	185	185	100	6.11	13.7	8.55	0.0607	0.0663
1.27 - 1.19	177	177	100	5.88	7.3	6.23	0.0743	0.0681
1.19 - 1.14	172	172	100	5.4	10.4	6.58	0.063	0.0688
1.14 - 1.08	210	210	100	5.4	3.5	4.5	0.1118	0.0978
1.08 - 1.03	221	221	100	5.15	3.4	3.77	0.1075	0.105
1.03 - 0.99	206	206	100	5.18	5.6	4.91	0.0866	0.088
0.99 - 0.96	191	191	100	4.71	4.3	3.53	0.1082	0.1153
0.96 - 0.93	173	173	100	4.7	6.2	4.15	0.0839	0.0925
0.93 - 0.9	253	253	100	4.67	3.8	3.49	0.1122	0.1151
0.9 - 0.87	257	258	99.6	4.66	3.2	3.19	0.1393	0.1317
0.87 - 0.85	174	174	100	4.55	1.3	1.93	0.2798	0.2461
0.85 - 0.83	244	244	100	4.41	2.4	2.92	0.1887	0.1735
0.83 - 0.8	259	259	100	3.86	1.7	2.37	0.2301	0.2334
Inf - 0.8	3428	3439	99.7	5.18	9.1	5.29	0.0602	0.0755

If the superstructure reflections, distinctly observable in the XRD patterns of $CsPbBr_3$ (Figure 1), are ignored from consideration, and only the reduced unit cell with V=795.2 Å^3 is considered, the crystal structure refinement in the orthorhombic *Pnma* symmetry would give relatively small *R*-factors, although, still yielding to the ones for $P2_1/m$ symmetry. For comparison, we present below Table S2 with data only for the substructure of $CsPbBr_3$ (the same massif, but ignoring the superstructural reflections) for the orthorhombic *Pnma* structure for the reduced unit cell with V=795.2 Å^3. As one can see, the R_{int} and R_{sigma} magnitudes in this case are comparable with those for monoclinic $P2_1/m$ symmetry in the above Table S1 for the double unit cell with V=1590.5 Å^3, based on the superstructural reflections.

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Table S2. Intensity statistics for XRD data for the substructure of $CsPbBr_3$ (*Pnma; V* = 795.2 Å^3).

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/σ	R(int)	Rσ
Inf - 2.25	51	52	98.1	7.85	82.4	16.59	0.0346	0.0481
2.25 - 1.75	54	54	100	10.39	54.3	18.18	0.0435	0.0498
1.75 - 1.52	51	51	100	10.69	31.4	19.01	0.0522	0.0433
1.52 - 1.37	53	53	100	11.13	26.4	14.31	0.0663	0.0481
1.37 - 1.27	59	59	100	10.51	32.7	16.45	0.0551	0.0446

1.27 - 1.19	54	54	100	10.81	22.4	15.51	0.0719	0.0446
1.19 - 1.14	53	53	100	9.25	16.9	13.04	0.0723	0.0458
1.14 - 1.08	53	53	100	9.68	7.4	10.59	0.0964	0.0566
1.08 - 1.03	66	66	100	8.89	6.2	8.33	0.1047	0.065
1.03 - 0.99	63	63	100	9.35	10.2	10.62	0.0978	0.0559
0.99 - 0.96	70	70	100	8.23	12.8	9.54	0.0778	0.0594
0.96 - 0.93	55	55	100	8.71	7.9	8.94	0.1054	0.0614
0.93 - 0.9	51	51	100	8.12	4.4	5.47	0.1153	0.0837
0.9 - 0.87	50	50	100	8.6	5.4	6.73	0.1297	0.0743
0.87 - 0.85	58	58	100	8.64	4.9	6.23	0.1374	0.0772
0.85 - 0.83	72	72	100	7.82	4.2	6.27	0.1528	0.0922
0.83 - 0.8	74	74	100	6.69	3.2	5.27	0.1811	0.1173
Inf - 0.8	987	988	99.9	9.05	18.5	10.96	0.0627	0.0519