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Electronic Supplementary Information

Time-Dependent Transformation Routes of Perovskites $CsPbBr_3$ and $CsPbCl_3$ under High Pressure

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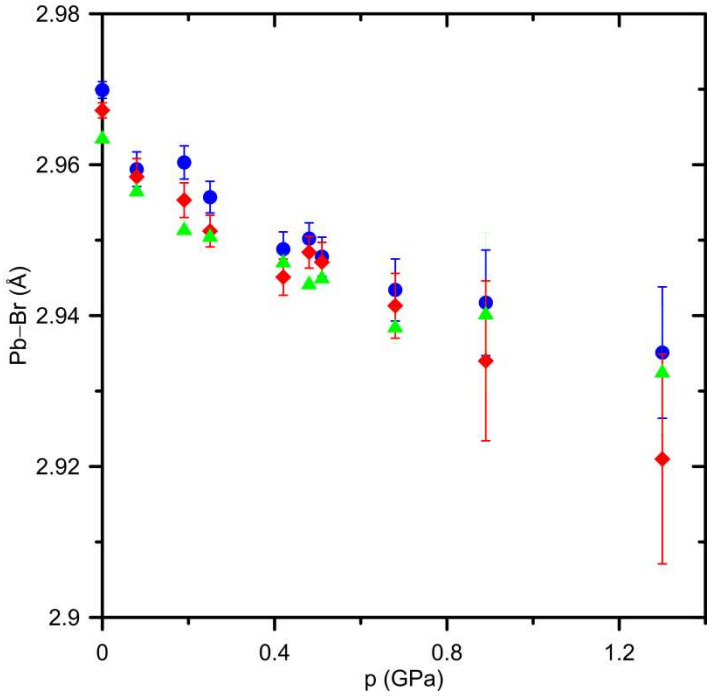

Fig. S1. Pressure dependence of Pb–Br distances in phase III of 3D-$CsPbBr_3$.

PXRD refinements summary

All refinements used the pseudo-Voigt profile function, where the *v* and *w* half-width parameters; one peak shape parameter were refined. The Chebyshev background function used 5-17 parameters. One or two preferred-orientation parameters were employed. No atomic parameters were refined.

Table S1. Refinement details for samples A, B and C (Figures S2–S4).

Sample no.	C	B	A	
Pressure	0.77 GPa	atm.	atm.	
Wavelength (Å)	0.70926/0.71354	1.54056	1.54056	
2θ-range/step size (°)	2.98-36.96/0.01	7.97-69.96/0.01	7.96-69.95/0.01	
Compound	1D-$CsPbBr_3$	1D-$CsPbBr_3$	1D-$CsPbBr_3$	$CsPb_2Br_5$
Space group	*Pmnb*	*Pmnb*	*Pmnb*	*I4/mcm*
R_p (%)	2.44	2.01	3.36	
R_{wp} (%)	3.59	2.83	7.28	
GOF	4.72	1.08	7.05	
R_B (%)	2.18	1.47	4.54	23.92
a (Å)	4.5651(12)	4.597(2)	4.5945(3)	8.4924(8)
b (Å)	9.576(2)	9.6976(5)	9.6986(7)	
c (Å)	16.614(5)	16.7768(7)	16.7770(9)	15.2070(8)

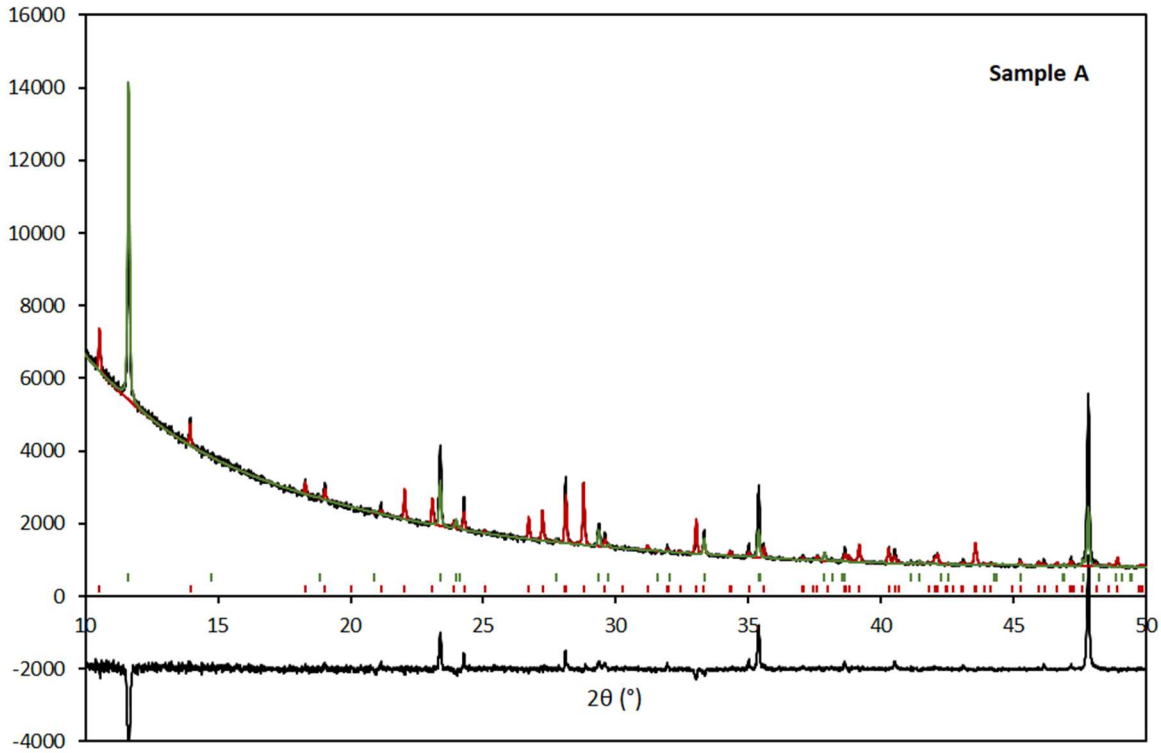

Fig. S2. PXRD of $CsPbBr_3$ after the transformation in isopropanol at o.60 GPa. The red and green markers show the positions of Bragg reflections for white 1D $CsPbBr_3$ and 2D $CsPb_2Br_5$. The bottom plot shows the (I_o-I_c) differences between the observed data (I_o) and the summed profiles (I_c) calculated for the white 1D $CsPbBr_3$ and 2D $CsPb_2Br_5$ structures retrieved from the ICSD.[40,41]

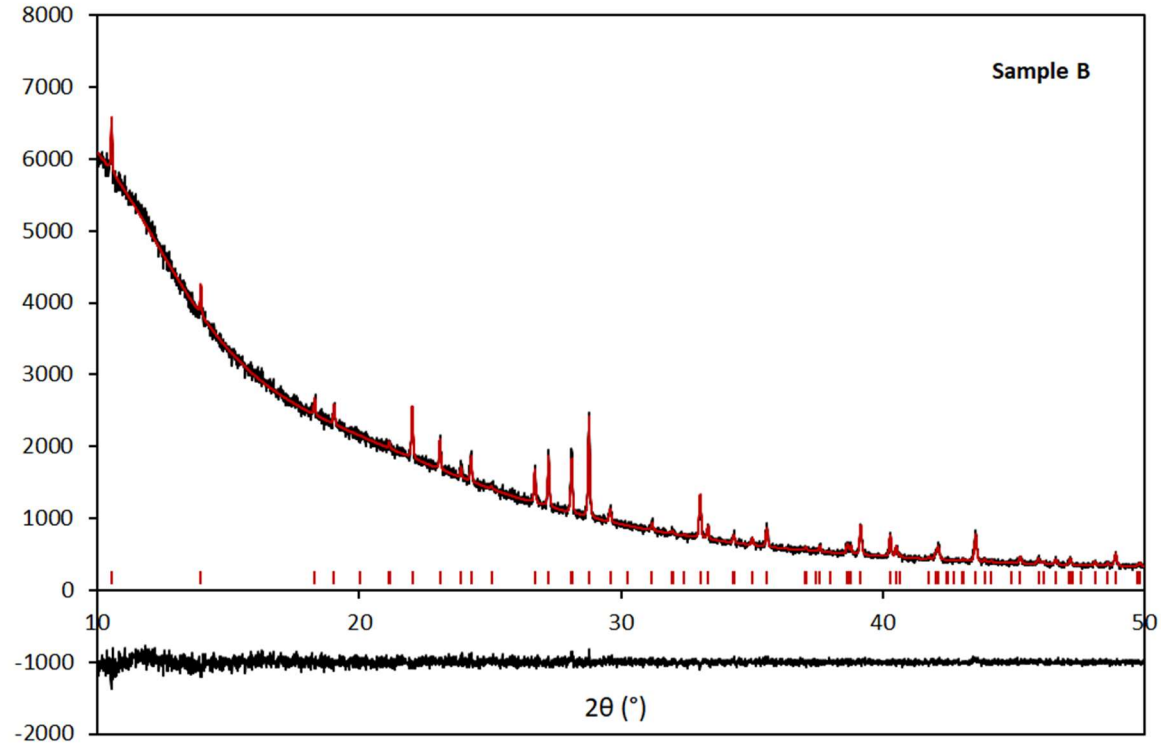

Fig. S3. PXRD of the $CsPbBr_3$ sample transformed under pressure of helium into the 1D form, as identified by the Rietveld refinement.

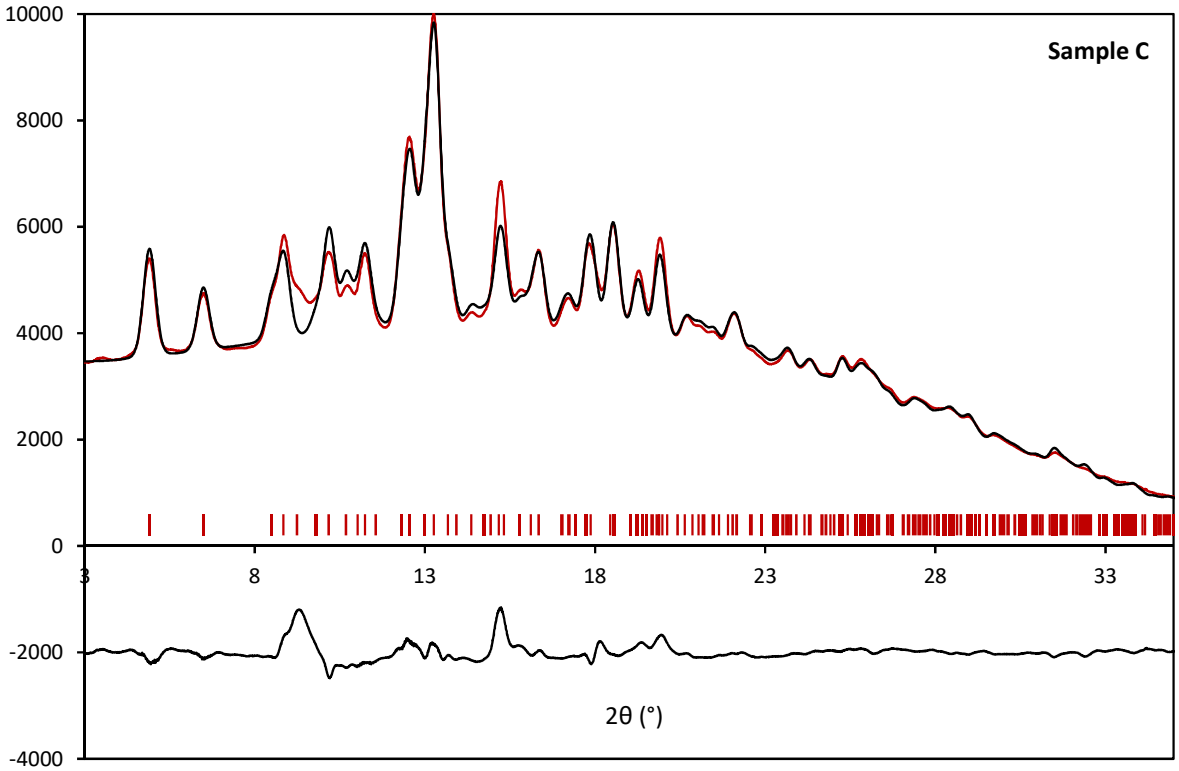

Fig. S4. PXRD of orange 3D-$CsPbBr_3$ phase III transformed under hydrostatic pressure in galden at 0.77 GPa during 2 weeks. The Rietveld refinement identifies the product as white 1D-$CsPbBr_3$ isomer.

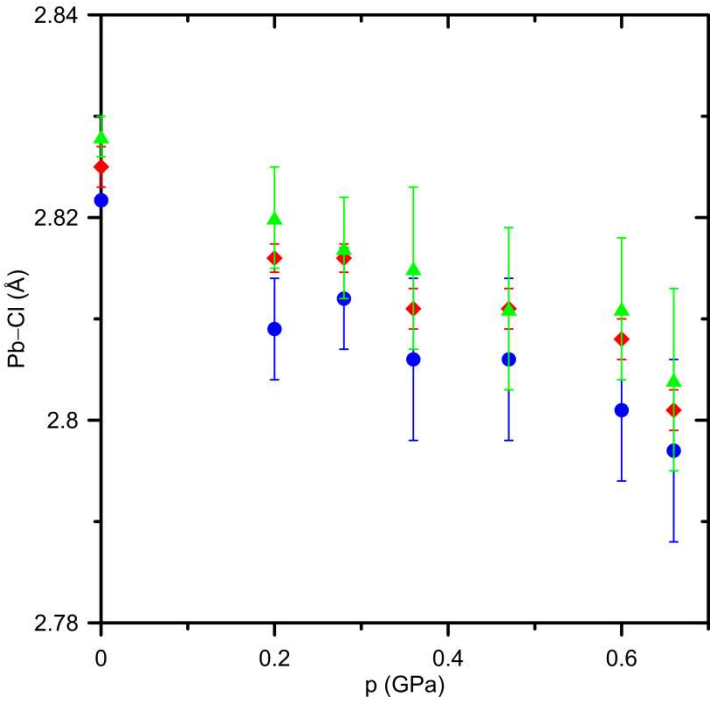

Fig. S5. Pressure dependence of Pb–Cl distances in phase IV of $CsPbCl_3$.

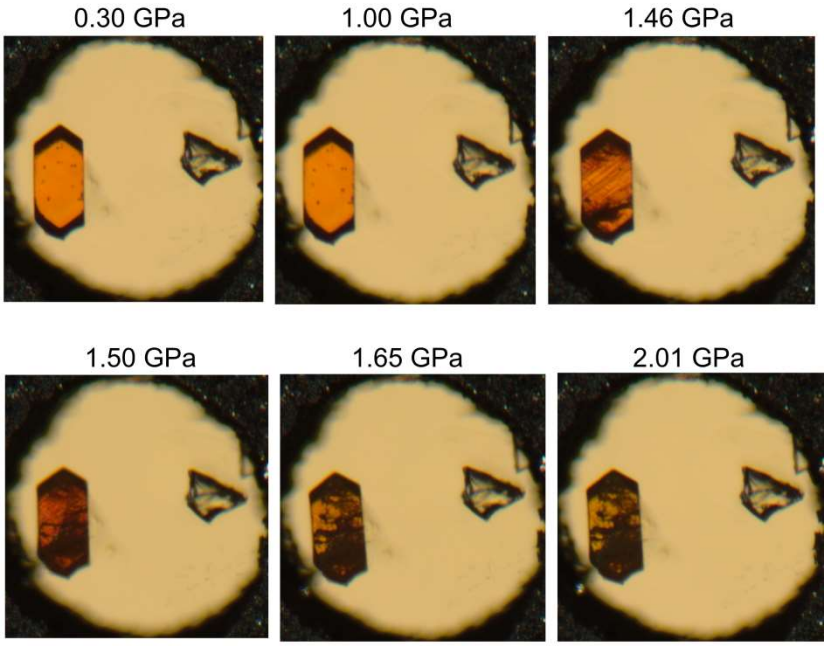

Fig. S6. Single crystal of orange 3D-$CsPbBr_3$ phase III quickly compressed in a DAC. Isopropanol was used as a hydrostatic liquid; a ruby chip for pressure calibration is placed close to the right edge of the DAC chamber.

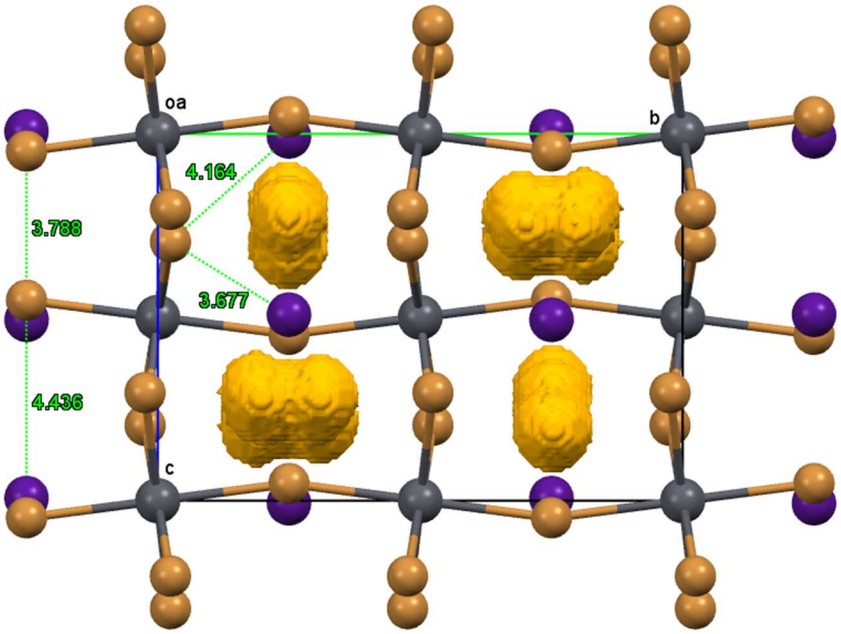

Fig. S7. Crystal structure of $CsPbBr_3$ phase III at ambient conditions, viewed along [x], with the voids (shown in gold) calculated for the probing radius 0.8Å and step 0.1 Å The shortest Br–Cs distances are indicated.