Supplementary Information

Phase Transitions, Screening and Dielectric Response of $CsPbBr_3$

Šarūnas Svirskas[1*], Sergejus Balčiūnas[1], Mantas Šimėnas[1], Gediminas Usevičius[1], Martynas Kinka[1], Martynas Velička[1], Dominik Kubicki[2], Marianela Escobar Castillo[3], Andrei Karabanov[3], Vladimir V. Shvartsman[3], Maria de Rosário Soares[4], Valdas Šablinskas[1], Andrei N. Salak[5], Doru C. Lupascu[3], Jūras Banys[1]

[1]*Faculty of Physics, Vilnius University, Sauletekio al. 9, LT-10222 Vilnius, Lithuania*

[2]*Institute of Chemical Sciences and Engineering, School of Basic Sciences, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland*

[3]*Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Essen, Germany*

[4]*Central Analytical Laboratory, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*

[5]*Department of Materials and Ceramics Engineering, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*

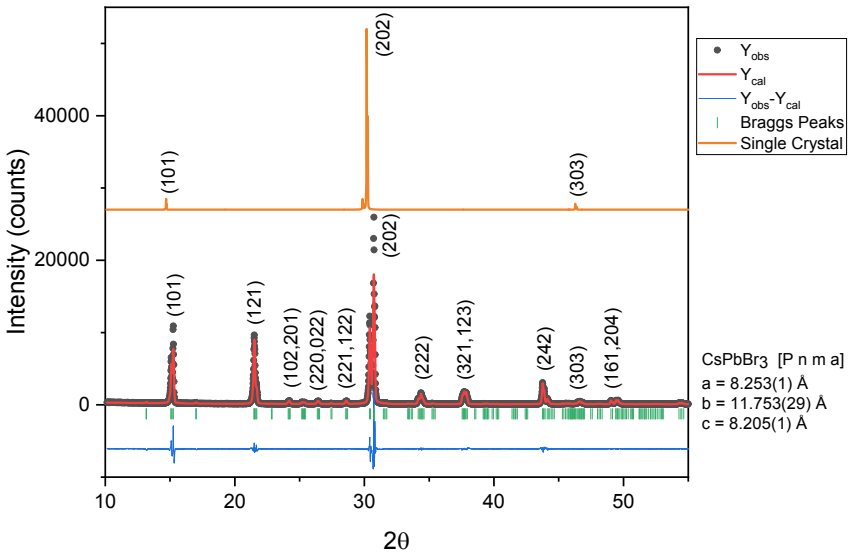

Figure S1. X-ray diffractogram of $CsPbBr_3$ single crystal.

Table S1. Selected crystallographic data for the annealed $CsPbBr_3$ powder sample obtained using the laboratory X-ray (T = **215 K**, Cu $K\alpha$ radiation, $\lambda\alpha_1$= 1.54053 Å, $\lambda\alpha_2$= 1.54431 Å) and refined in the ***Pnma*** space group ($\sqrt{2}a_p \times 2a_p \times \sqrt{2}a_p$ superstructure).

Chemical formula	$CsPbBr_3$
Formula weight ($g \cdot mol^{-1}$)	579.81
Crystal system	Orthorhombic
Space group (No.)	*Pnma* (62)
a (Å)	8.2745(3)
b (Å)	11.7116(3)
c (Å)	8.1249(3)
V (Å^3)	787.375(44)
Z	4
d-space range (Å)	7.3539 - 1.6685
χ^2	2.85
R_p (%)	3.14
R_{wp} (%)	4.25

For definition of the agreement factors χ^2, R_p and R_{wp} see Ref. [1].

Table S2. Selected crystallographic data for the annealed $CsPbBr_3$ powder sample obtained using the laboratory X-ray (T = **210 K**, Cu $K\alpha$ radiation, $\lambda\alpha_1$= 1.54053 Å, $\lambda\alpha_2$= 1.54431 Å) and refined in the ***Pnma*** space group ($\sqrt{2}a_p \times 2a_p \times \sqrt{2}a_p$ superstructure).

Chemical formula	$CsPbBr_3$
Formula weight ($g \cdot mol^{-1}$)	579.81
Crystal system	Orthorhombic
Space group (No.)	*Pnma* (62)
a (Å)	8.2819(3)
b (Å)	11.7153(3)
c (Å)	8.1209(2)
V (Å^3)	787.939(42)
Z	4
d-space range (Å)	7.3539 - 1.6685
χ^2	2.83
R_p (%)	3.03
R_{wp} (%)	4.09

For definition of the agreement factors χ^2, R_p and R_{wp} see Ref.[1]

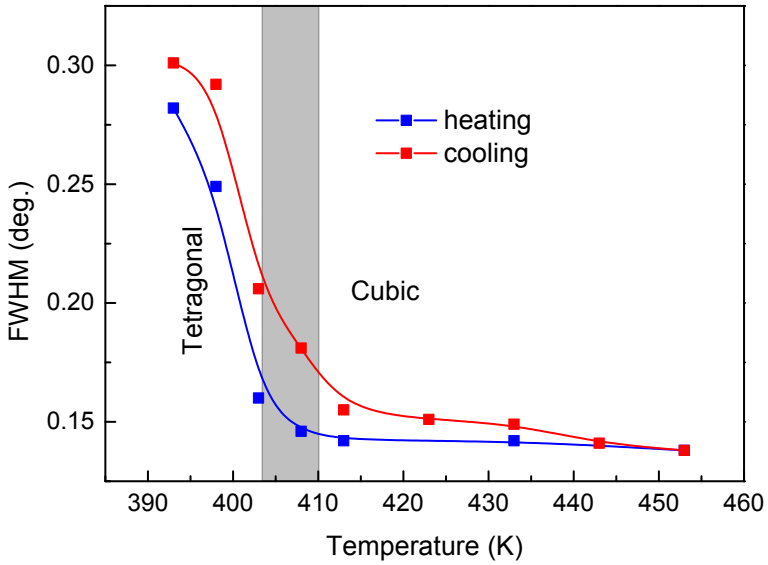

Figure S2. Full width at half maximum (FWHM) of the $(002)_p$ multiplet in the XRD patterns of $CsPbBr_3$ in the vicinity of the *Pbnm* - *P*4/*mbm* phase transition recorded upon heating and upon cooling.

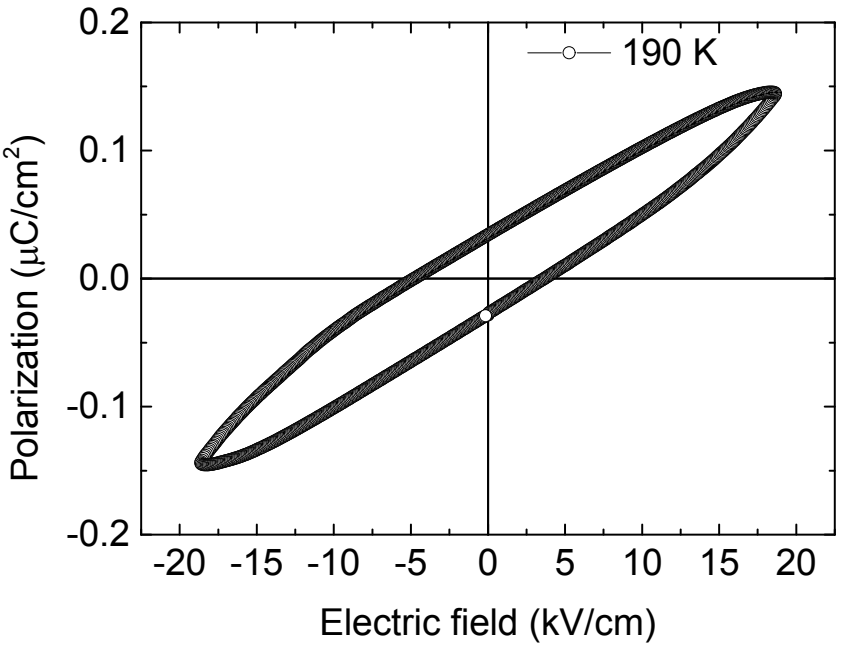

Figure S3. Electric field dependence of polarization on electric field at T = 190 K.

Figure S3 represents the electric field dependence of polarization in $CsPbBr_3$ single crystal at 190 K temperature. It is evident that no polarization switching is observed up to 20 kV/cm.

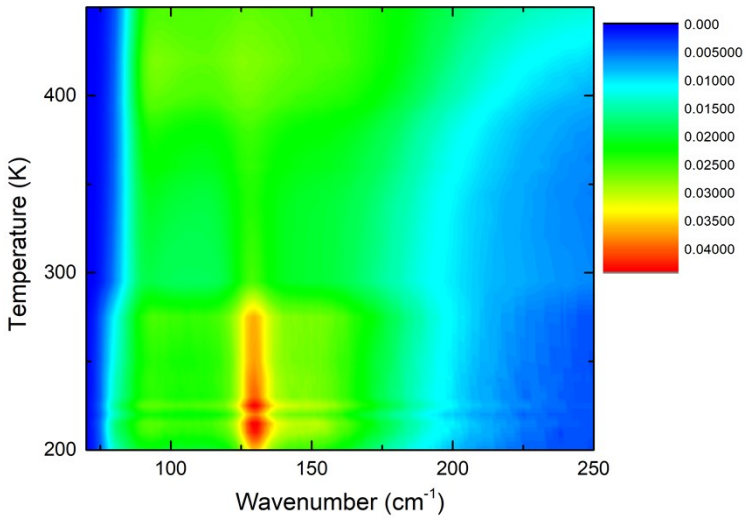

Figure S4. Raman scattering spectra of $CsPbBr_3$ at different temperatures.

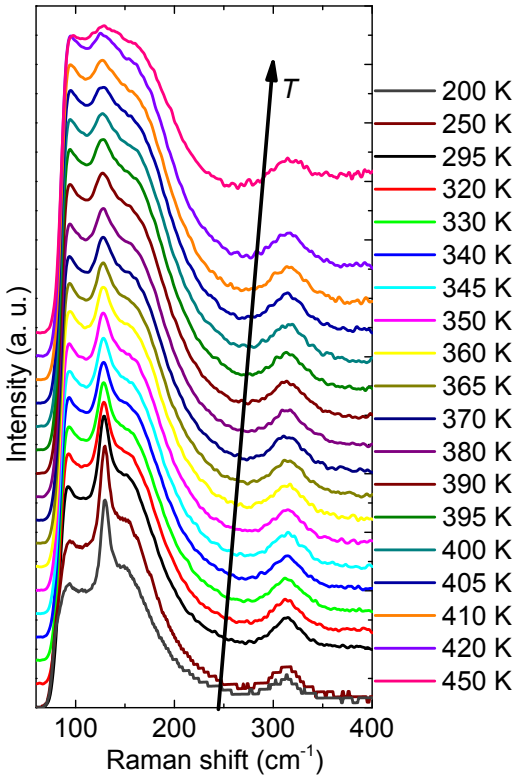

Figure S5. Raman scattering spectra of $CsPbBr_3$ at different temperatures.

References

[1] J. Rodríguez-Carvajal, Physica B: Condensed Matter **192**, 55 (1993).