Size-tunable and stable cesium lead-bromide perovskite nanocubes with near-unity photoluminescence quantum yield

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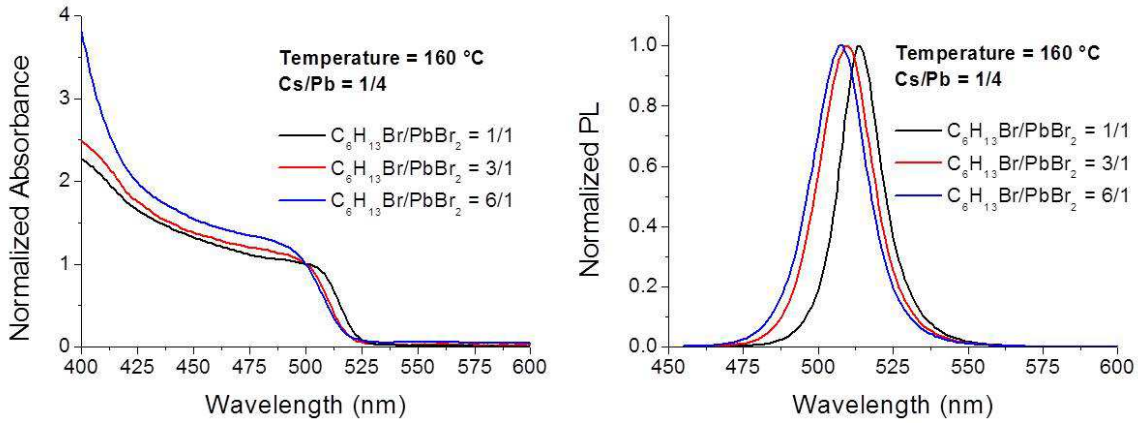

Figure 1S. *(left) Normalized (λ = 500 nm) absorption spectra (cyclohexane) of the $CsPbBr_3$ NCs synthesized at 160 °C and a fixed Cs/Pb molar ratio (1/4) with different $C_6H_{13}Br/PbBr_2$ molar ratios. (right) Normalized PL spectra (cyclohexane) of the same NCs.*

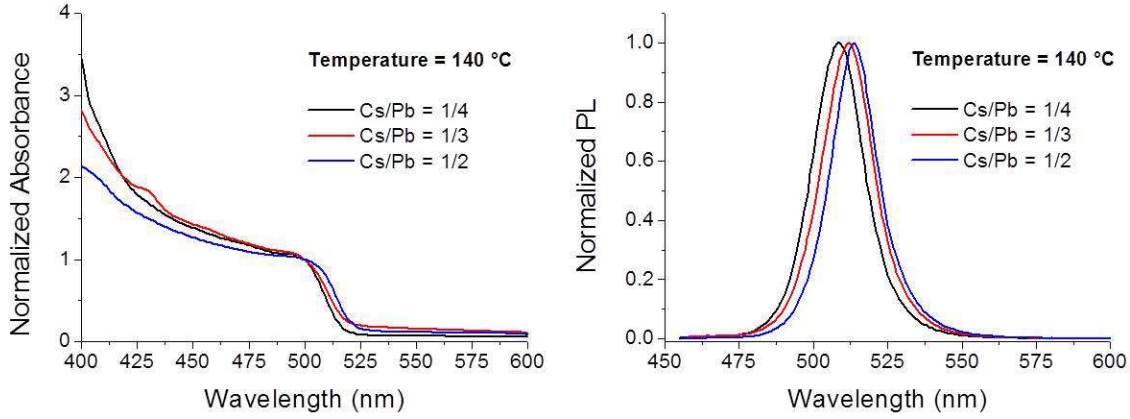

Figure 2S. *(left) Normalized (λ = 500 nm) absorption spectra (cyclohexane) of the $CsPbBr_3$ NCs synthesized at 140 °C with different Cs/Pb molar ratios and (right) the corresponding photoluminescence profiles recorded in cyclohexane.*

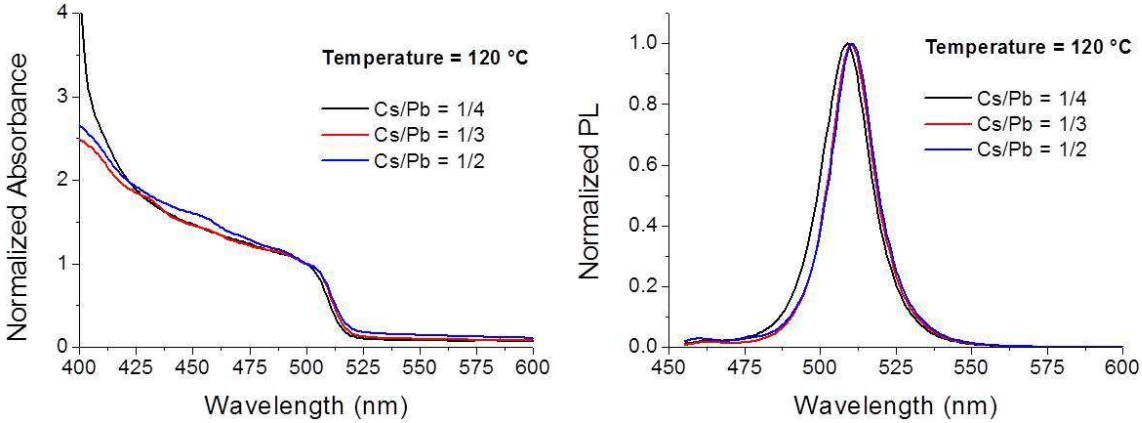

Figure 3S. *(left) Normalized (λ = 500 nm) absorption spectra (hexane) of the $CsPbBr_3$ NCs synthesized at 120 °C with different Cs/Pb molar ratios and (right) the corresponding photoluminescence profiles recorded in cyclohexane.*

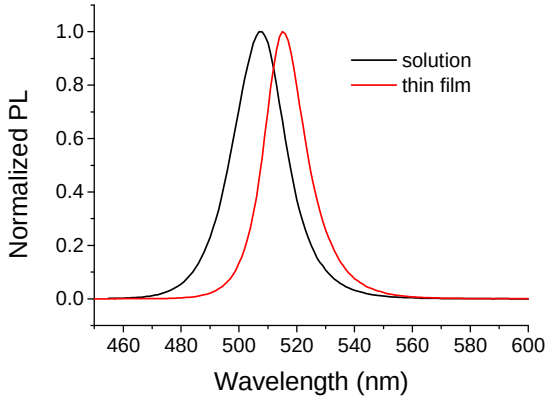

Figure 4S. *Normalized PL spectra of the $CsPbBr_3$ NCs synthesized at 160 °C with Cs/Pb molar ratio of 1/4 in cyclohexane and in the solid state.*

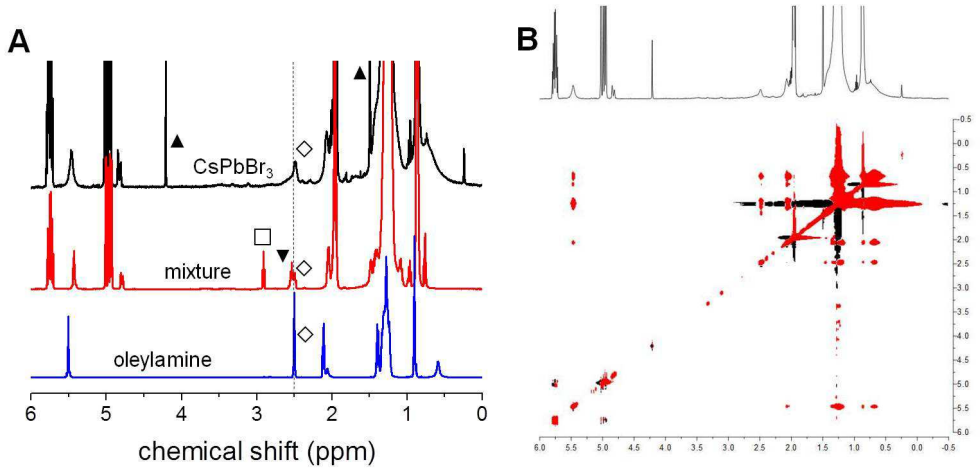

Figure 5S. *(A) Comparison between the ^{1}H-NMR spectra (benzene-d_6) of $CsPbBr_3$ NCs, the reaction mixture constituted by $PbBr_2$, oleylamine and 1-bromohexane in ODE kept at 160 °C for 30 min and pure oleylamine. The plot highlights the characteristic resonances of the secondary amine (–C**H**$_2$NH–, ▼), of oleylamine (–C**H**$_2$NH$_2$, ◊) and of residual 1-bromohexane (–C**H**$_2$Br, □). The resonances ▲ are associated to methyl acetate used for the purification of the NCs. (B) NOESY spectrum of the aforementioned $CsPbBr_3$ NCs in benzene-d_6.*

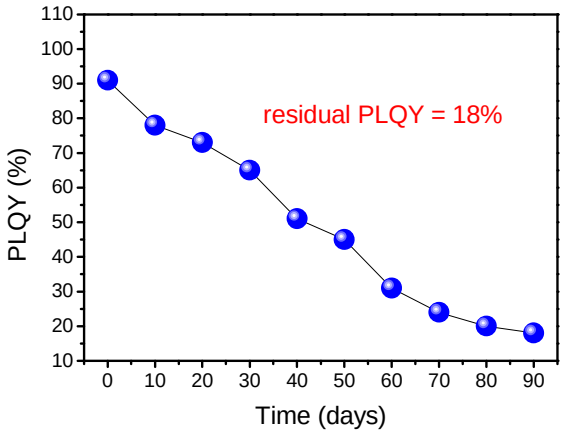

Figure 6S. *PLQY trend as a function of time (days) for the cyclohexane solution of the NC synthesized in the presence of oleic acid.*

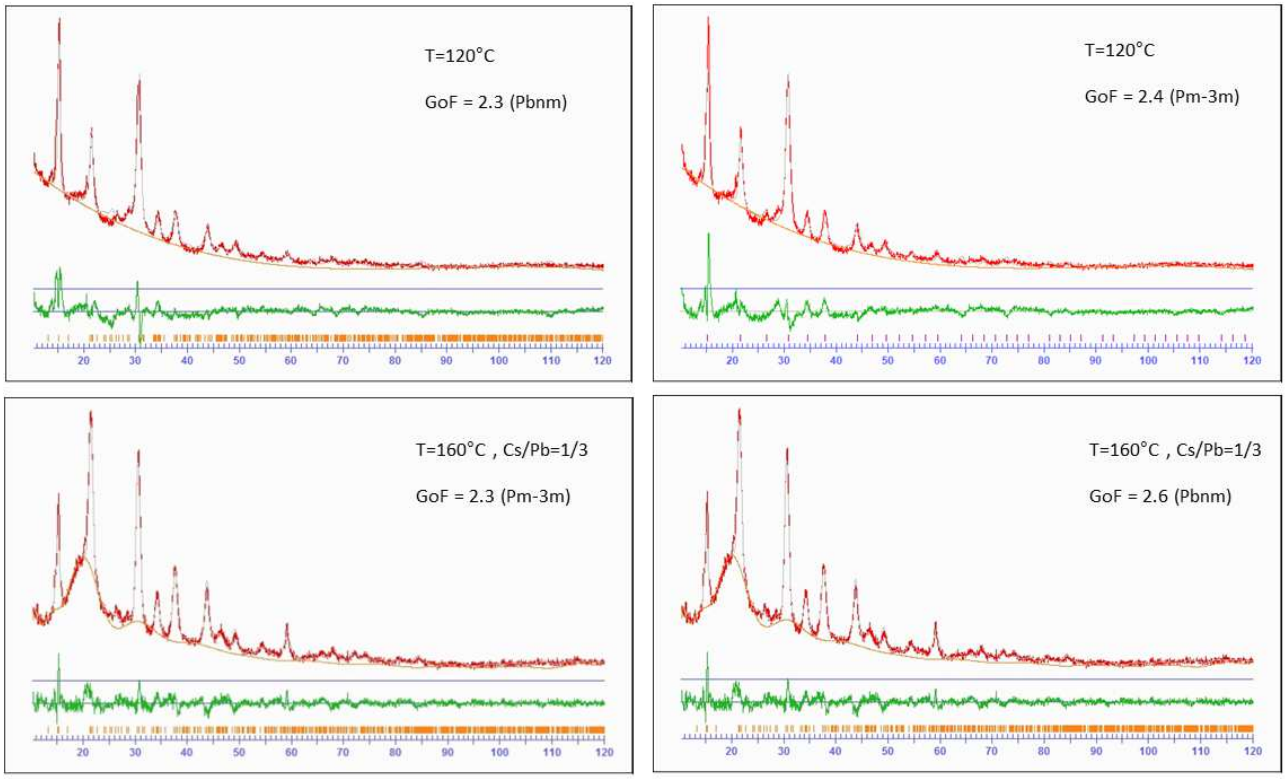

Figure 7S. *XRD experimental (detector scan, 5° incidence, red curves) and relevant fit profiles (orange curves) are reported for samples prepared at T=120 °C and T = 160 °C with Cs/Pb = 1/3. Fitting was based on the orthorhombic (Pbnm space group) or cubic (Pm-3m) $CsPbBr_3$ structure model (ICSD-97851 and COD-1533063, respectively). The difference profile (green curve) and the expected peak positions (bars) are reported at the bottom of each panel. Fits featuring the lower GoF value are reported on the left column.*

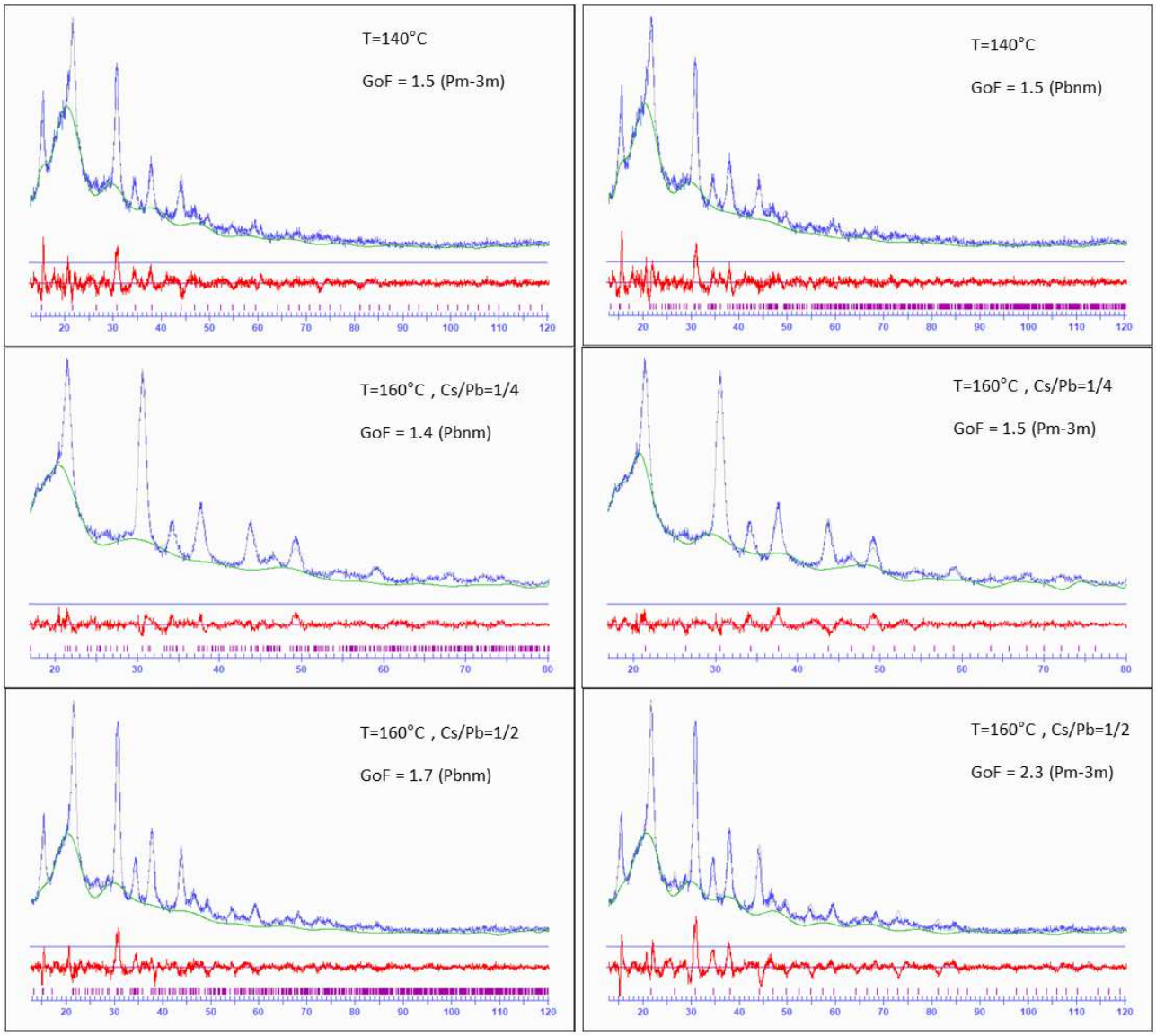

Figure 8S. *XRD experimental (detector scan, 5° incidence, blue curves) and relevant fit profiles (grey lines) are reported for samples prepared at T=140 °C and T = 160 °C with Cs/Pb = 1/4 and Cs/Pb = 1/2. Fitting was based on the orthorhombic (Pbnm) or cubic (Pm-3m) $CsPbBr_3$ structure model (ICSD-97851, COD-1533063, respectively). The difference profile (red curve) and the expected peak positions (bars) are reported at the bottom of each panel. Fits featuring the lower GoF value are reported on the left column.*