Room Temperature Synthesis and Characterization of Novel Lead-free Double Perovskite Nanocrystals with a Stable and Broadband Emission

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Fig. S1. (a) XRD patterns for precursor ratios of CsBr and BiBr$_3$ at 1.5:1 and 3:1 compared to simulated Cs$_3$Bi$_2$Br$_9$ and Cs$_3$BiBr$_6$ XRD pattern. (b) UV spectra of the Cs$_3$Bi$_2$Br$_9$ NCs.

Fig. S2. (a) HAADF-STEM image for Cs$_3$BiBr$_6$-5.5 NCs, the inset is the size distribution. (b) HAADF-STEM image for Cs$_3$BiBr$_6$-10 NCs, the inset is the size distribution. (c) HAADF-STEM image for Cs$_3$BiBr$_6$-10 NCs. (d) HRTEM image for Cs$_3$BiBr$_6$-10 NC with a lattice fringe of 0.22 nm.
Fig. S3. (a) Comparison of XRD patterns with the simulated XRD patterns of precursors (CsBr-1, \(Fm-3m\); CsBr-2, \(Pm-3m\); BiBr\(_3\), \(P2_1/c\)), Cs\(_3\)BiBr\(_6\) and Cs\(_3\)BiBr\(_6\)-5.5 NCs. (b) Zoom-in of the XRD pattern of Cs\(_3\)BiBr\(_6\)-7.5, Cs\(_3\)BiBr\(_6\)-10, Cs\(_3\)BiBr\(_6\)-20 NCs.

Fig. S4. XPS characteristics for Cs\(_3\)BiBr\(_6\)-5.5 NCs: (a) Survey spectra; b) Cs 3d; c) Bi 4f; d) Br 3d. For Cs 3d electrons, the two peaks centred at 724.4 eV and 738.4 eV correspond to the Cs 3d\(_{5/2}\) and Cs 3d\(_{3/2}\) states with a spin-orbit splitting of 14 eV. Similarly, in the Br 3d spectra, peaks at 68.1 eV and 69.3 eV are assigned to Br 3d\(_{5/2}\) and Br 3d\(_{3/2}\), with a well-resolved spin-orbit splitting of ~1.2 eV, while in the Bi 4f spectra, two peaks located at 159.2 eV and 164.6 eV, with a spin-orbit splitting of 5.4 eV, can be observed.
**Fig. S5.** Absorption spectra for Cs$_3$BiBr$_6$ NCs synthesized at 70 °C.

**Fig. S6.** Tauc’ plot for Cs$_3$BiBr$_6$ NCs.
Fig. S7. (a) PL contour map for OA ligands. (b) Cs$_3$BiBr$_6$ NCs with OA ligands.

Fig. S8. Gaussian fitting with three peaks: excitation peak, OA-ligand related peak and Cs$_3$BiBr$_6$-related emission for PL emission of Cs$_3$BiBr$_6$ NCs at 150 K.
Fig. S9. PL spectra for Cs$_3$BiBr$_6$ NCs at room temperature before and after three weeks by an excitation wavelength of 355 nm.

Table S1. Crystal data and structure refinements for the Cs$_3$BiBr$_6$ at 120 K.

| formula | Cs$_3$BiBr$_6$ |
|---------|---------------|
| fw      | 1087.17       |
| T, K    | 120 K         |
| $\lambda$, Å | 0.71073     |
| Space group | $Pbcm$       |
| a, Å    | 8.637(3)      |
| b, Å    | 13.495(6)     |
| c, Å    | 27.532(6)     |
| $\alpha$, deg | 90            |
| $\beta$, deg | 90           |
| $\gamma$, deg | 90           |
| V, Å³   | 3209.3(5)     |
| Z       | 8             |
| $D_{calcd}$, g cm$^{-3}$ | 4.500        |
| $\mu$, mm$^{-1}$ | 32.59        |
| GOF on $F^2$ | 1.345        |
| R1, wR2($|>2\sigma(|I|)$ | 0.0691, 0.1703 |
| R1, wR2(all data) | 0.0806, 0.1745 |