SUPPORTING INFORMATION

Microwave-mediated Synthesis of Lead-Free Cesium Titanium Bromide Double Perovskite: A Sustainable Approach

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Figure S6. a) XPS spectra of the Cs_2TiBr_6 powder exhibit a high level of resolution for a) Cs *3d*, b) Ti *2p*, c) Br *3d*, and d) O *1s* (including deconvolution of the different oxygen species present in the sample).

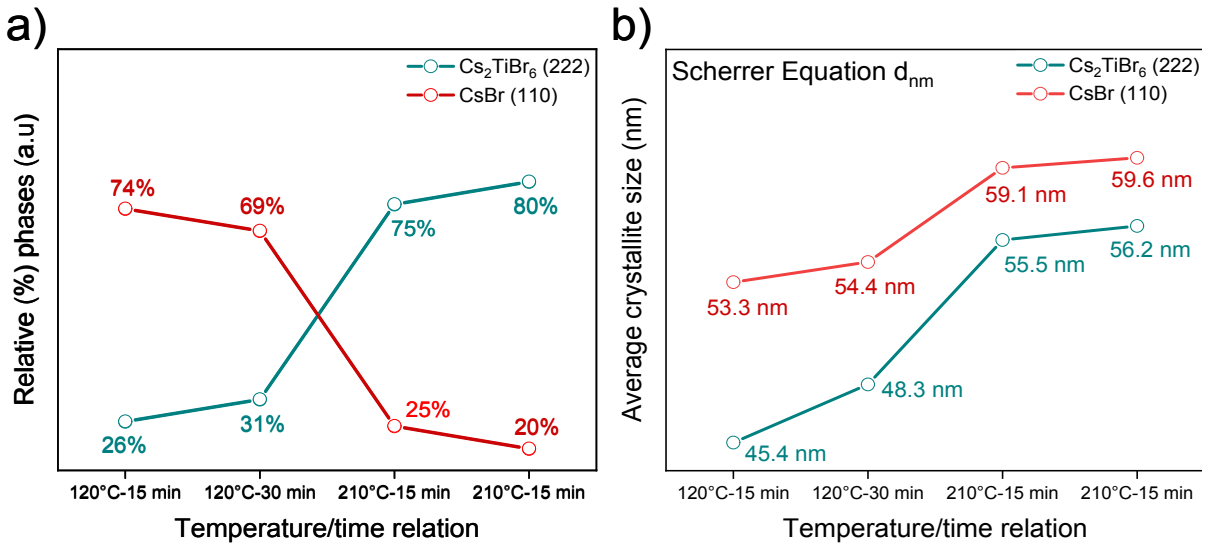


Figure S1. a) Relative mass percentages calculated from XRD patterns (*) and b) average crystallite size (extracted from Scherrer equation) for the Cs_2TiBr_6 and CsBr phases analyzed at different conditions of MW-reaction temperature and time.

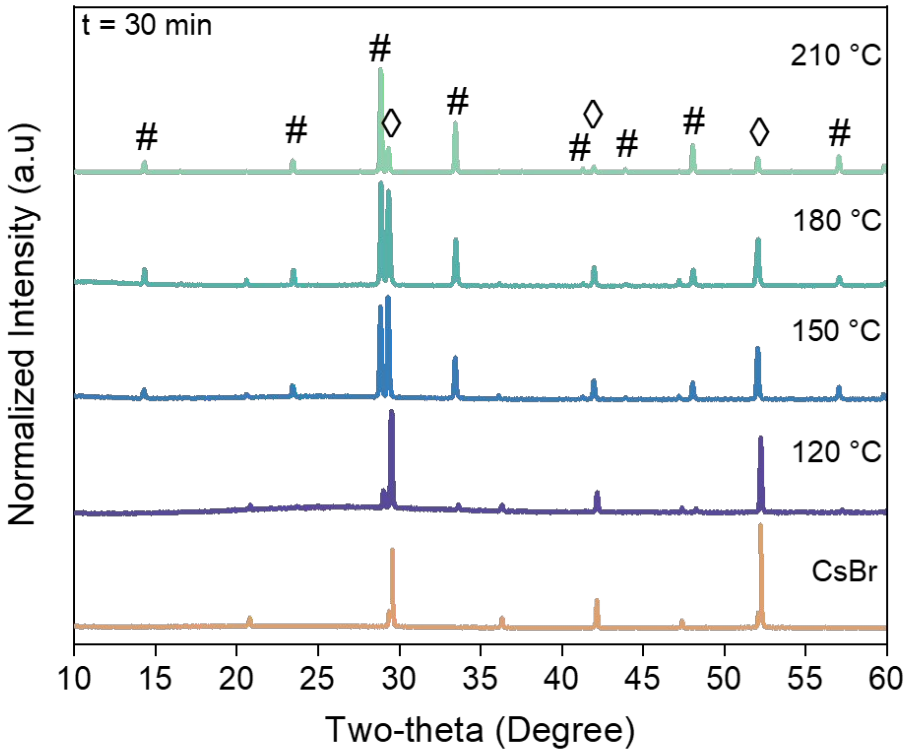
(*) X-ray diffraction technique allows quantitative analysis of a crystalline phase (component P) in a solid sample by adding an internal standard s (internal standard method [1]). The formula developed by Alexander and Klug is:

$$x_p = kI_p/I_s$$

where k is a coefficient related to the nature of component P and internal standard s, to properties of the X-ray diffraction measurement (i.e., the geometry of the apparatus and the wavelength of the X-ray) and to the amount added from the standard. x_p is the mass % of component P. I_p and I_s are the X-ray diffraction intensities of the more intense hkl peaks of component P and the standard s, respectively.

For the quantitative analysis of our binary mixtures composed of Cs_2TiBr_6 and CsBr, we prepared a set of samples using corundum as standard and CsBr as component P. The experimental XRD patterns provided us with the intensities of the peaks of corundum and CsBr (we considered (104) and (110) planes, respectively) and k was extracted from the equation. Then, we added 10% mass of corundum to our binary mixtures and, with the experimental peak intensities and k, we calculated the mass % of CsBr (x_{CsBr}). The mass % of Cs_2TiBr_6 was directly inferred because $x_{Cs2TiBr6} + x_{CsBr} = 1$ (or 100 % in percentage). The representation of the mass % of both phases is given in Figures S1 and S3.

[1] L. Alexander, H.P. Klug, Basic aspects of X-ray absorption in quantitative diffraction analysis of powder mixtures, Anal. Chem., 20 (1948), 886-889.



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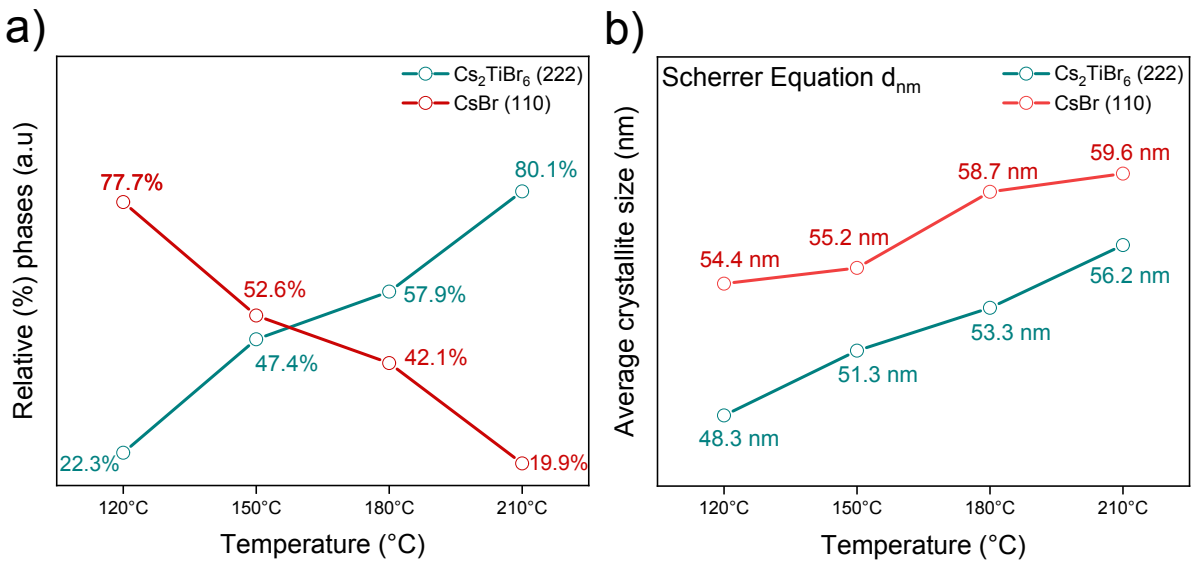

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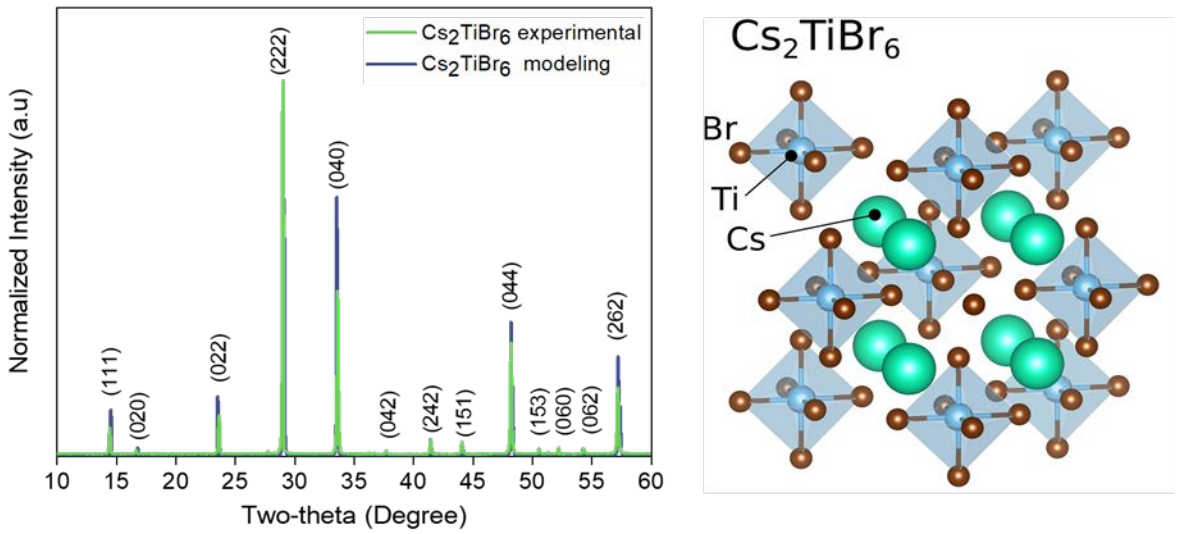

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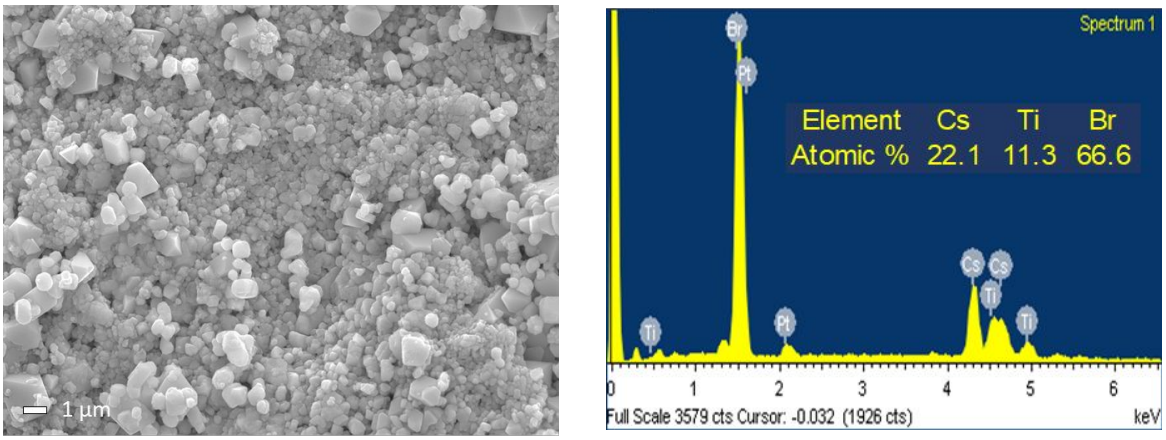
a) b)



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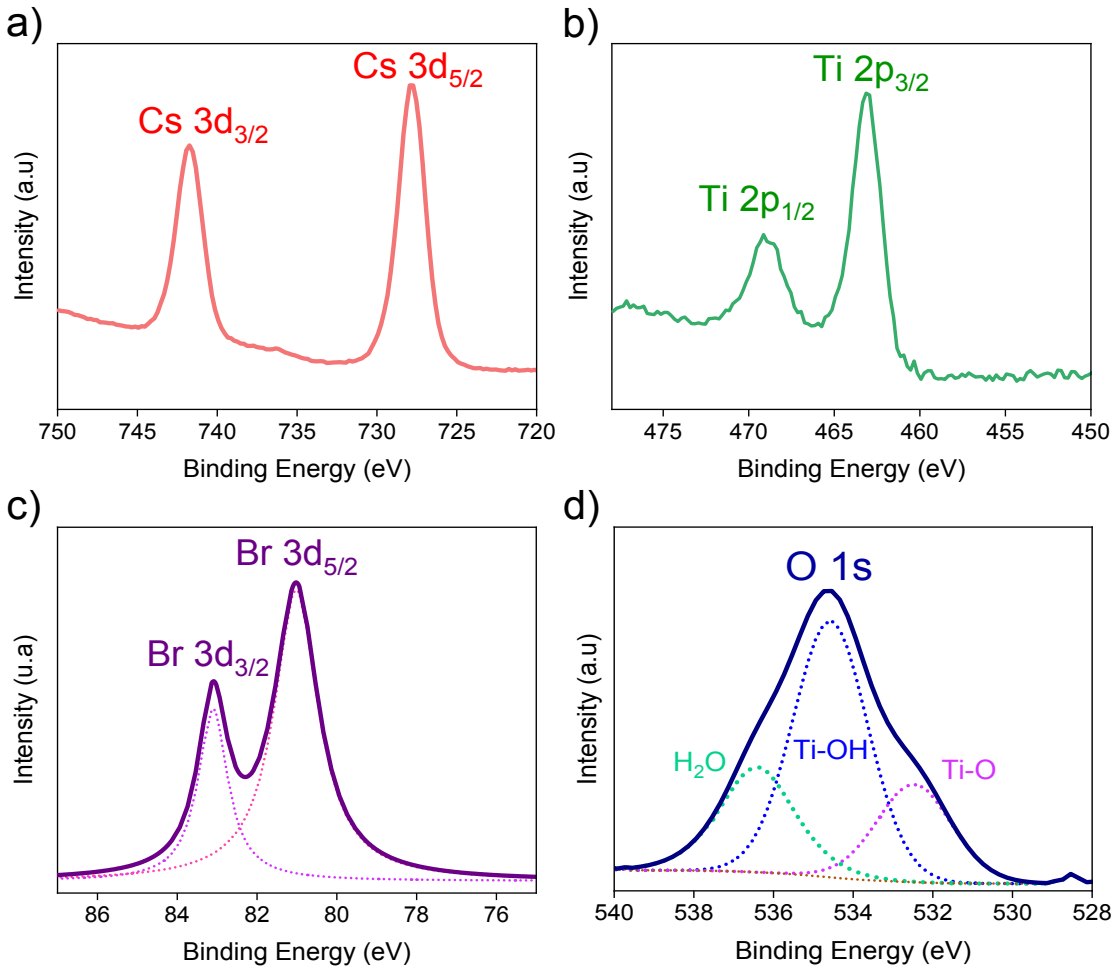

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