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High-Resolution In-situ Synchrotron X-ray Studies of Inorganic Perovskite $CsPbBr_3$: New Symmetry Assignments and Structural Phase Transitions. SIZHAN LIU, ALEXANDER DEFILIPPO, New Jersey Inst of Tech , MAHALINGAM BALASUBRAMANIAN , Argonne National Laboratory, ZHENXIAN LIU, University of Illinois at Chicago, SUYIN GRASS WANG, YU-SHENG CHEN, STELLA CHARITON, VITALI PRAKAPENKA , University of Chicago, JOVAN SAN MARTIN , YIXIONG LIN , YONG YAN, San Diego State University, SANJIT GHOSE , Brookhaven National Laboratory, TREVOR TYSON, New Jersey Inst of Tech — Perovskite photovoltaic systems are being studied due to their high energy conversion efficiencies with current emphasis on pure inorganic systems such as $CsPbBr_3$. In light of the inconsistency of existing space group assignments with recent experiments on this perovskite, high-resolution in-situ synchrotron single-crystal X-ray diffraction and local structure measurements complemented by optical and calorimetric measurements are used to explore the changes in atomic structure for temperatures between 100 and 500 K. The currently accepted space group assignments for $CsPbBr_3$ are found to be incorrect in a manner that profoundly impacts physical properties. The newly observed structural distortions of the bulk structure are consistent with the expectation of previous photoluminescence and Raman measurements. The new derived orthorhombic structure supports can support a ferroelectric state below room temperature. Multiple low-pressure phases are found, one of which exists as a metastable phase at ambient pressure. This work is supported by NSF Grant No. DMR-1809931.

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