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High pressure study of mixed valence compound CsAuI₃ SHIBING WANG, SHIGETO HIRAI, ALEXANDER KEMPER, Stanford University, MARIA BALDINI, Geophysical Laboratory, HONGWEI MA, Indiana University, SCOTT RIGGS, MAXWELL SHAPIRO, TOM DEVEREAUX, IAN FISHER, WENDY MAO, TED GEBALLE, Stanford University — CsAuI₃, chemically described as $Cs_2Au^IAu^{III}I_6$, is a mixed valence compound in the family of $CsAuX_3$ (X = Cl, Br, I), resembling the high Tc superconductor parent compound BaBiO₃. At ambient conditions it adopts a distorted perovskite structure with compressed $Au^{I}X_{6}$ octahedra and elongated $Au^{III}X_6$ octahedra along the crystallographic c-axis. The compound undergoes a pressure-induced transition into a new tetragonal phase comprising nearly equivalent AuX_6 octahedra around 5.3 GPa, which agrees with the valence transition previously reported using Mössbauer spectroscopy between 8-12 GPa. We present a thorough high pressure studies of CsAuI3 through X-ray diffraction and Raman spectroscopy, confirming a pressure-induced band Jahn-Teller effect associated with the $5d^9 Au^{II}$ ion. We will also report the reversible amorphization above 15 GPa.

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