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Inelastic X-ray scattering study of incipient and realized structural transitions in mercurous halides CONNOR OCCHIALINI, University of Connecticut, Storrs, CT, AYMAN SAID, AHMET ALATAS, Advanced Photon Source, Argonne National Lab, Argonne, IL , SUDHIR TRIVEDI, Brimrose Technologies Corporation, Sparks, MD, JASON HANCOCK, University of Connecticut, Storrs, CT — We present new x-ray scattering investigations of mercury halides Hg_2X_2, where X=I,Br in an effort to compare lattice dynamics and structural properties of an incipient (X=I) and realized (X=Br) structural phase transition. For the realized structural transition in Hg_2Br_2, we find mode softening centered on the X point in the high-temperature body-centered tetragonal Brillouin zone in a realized transition to a lower-symmetry orthorhombic phase below $T_c \simeq$140 K. For the incipient transition in Hg_2I_2, we also find dramatic mode softening along the Γ-X direction, implying a putative transition temperature of T_c=-22K. In addition, we report the first temperature dependent lattice parameter development in these two systems, and compare these structural properties of the mercurous halides (Hg_2X_2) with $3d$ transition metal trifluorides (XF_3), which host novel phases including negative thermal expansion.

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