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First-principles calculations of phonons and Raman spectra in monoclinic $CsSnCl_3$ LING-YI HUANG, WALTER LAMBRECHT, Case Western Reserve Univ — Halide perovskites have recently attracted attention for photovoltaic applications. While $CsSnCl_3$ in the perovskite structure is less suitable for solar cells because of its higher band gap than the iodides, it is still of interest as the end member of mixed $CsSn(I_{1-x}Cl_x)_3$ and addition of Cl has been found to increase solar cell efficiencies. The other reason this material is interesting is that at 390 K it undergoes a phase transition to a monoclinic structure with even larger band gap, which differs from the yellow phase occuring for $CsSnI_3$. Understanding the various possible phase transitions and structures in the trihalides is important for the long-term stability of these materials in solar cells. Raman data exist on monoclinic $CsSnCl_3$ material since the late 80s but have in the past not been compared with first-principles calculations of the phonons in this material. We present calculations of the phonons at the Γ-point using density functional perturbation theory using the abinit program. A symmetry analysis is presented and the calculated phonon modes are compared with experimental data and previous attempts to classify the modes as internal to the $SnCl_3$ tetrahedra and lattice modes. Supported by DOE.

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