

W0328

Crystal Structure of Methylammonium Lead Chloride & Methylammonium Tin Bromide: Low Temperature Phase of Perovskite Structure. Jae-Hyuk Her, Lisheng Chi, Ian Swainson, Lachlan Cranswick, Peter Stephens, Physics, Stony Brook Univ., Suffolk, Stony Brook, NY 11794.

The low temperature perovskite crystal structures of methylammonium (CH_3NH_3 ; MeAm) lead chloride and MeAm tin bromide were solved with X-ray powder diffraction (XRPD) method. The MeAmPbCl_3 orders into orthorhombic unit cell ($a=11.1747(5)\text{\AA}$, $b=11.3552(5)\text{\AA}$, $c=11.2820(5)\text{\AA}$, Volume= $1431.6(2)\text{\AA}^3$, at 80K) whose axes are doubled with respect to its room temperature aristotype cubic phase. The high resolution of synchrotron data revealed that the previously assigned unit cell information was wrong, and correct space group $\text{Pnma}(\#62)$ was determined according to the systematic absences. The structure was solved by direct method program EXPO and Rietveld-refined by program GSAS. The result shows highly distorted PbCl_6 octahedra, implying that the most rigid unit in that perovskite cell is the methylammonium cation.

In the MeAmSnBr_3 , we identified the room temperature aristotype phase and solved the structure of an orthorhombic ($\text{Pm}21b$; $a=5.8934(2)\text{\AA}$, $b=8.2510(2)\text{\AA}$, $c=8.3965(2)\text{\AA}$) phase at 200K with same experimental method and analysis tool. Below 30K, the lattice turned to triclinic ($\text{P}1$; $a=5.8979(2)\text{\AA}$, $b=8.1258(2)\text{\AA}$, $c=8.3411(2)\text{\AA}$, $\alpha=91.37(1)^\circ$, $\beta=89.86(1)^\circ$, $\gamma=92.12(1)^\circ$). Substantial hysteresis between two hettotype phases was also observed.