Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic supporting information for paper

Pyrrolidinium containing perovskites of thermal stability and water resistance for photovoltaics

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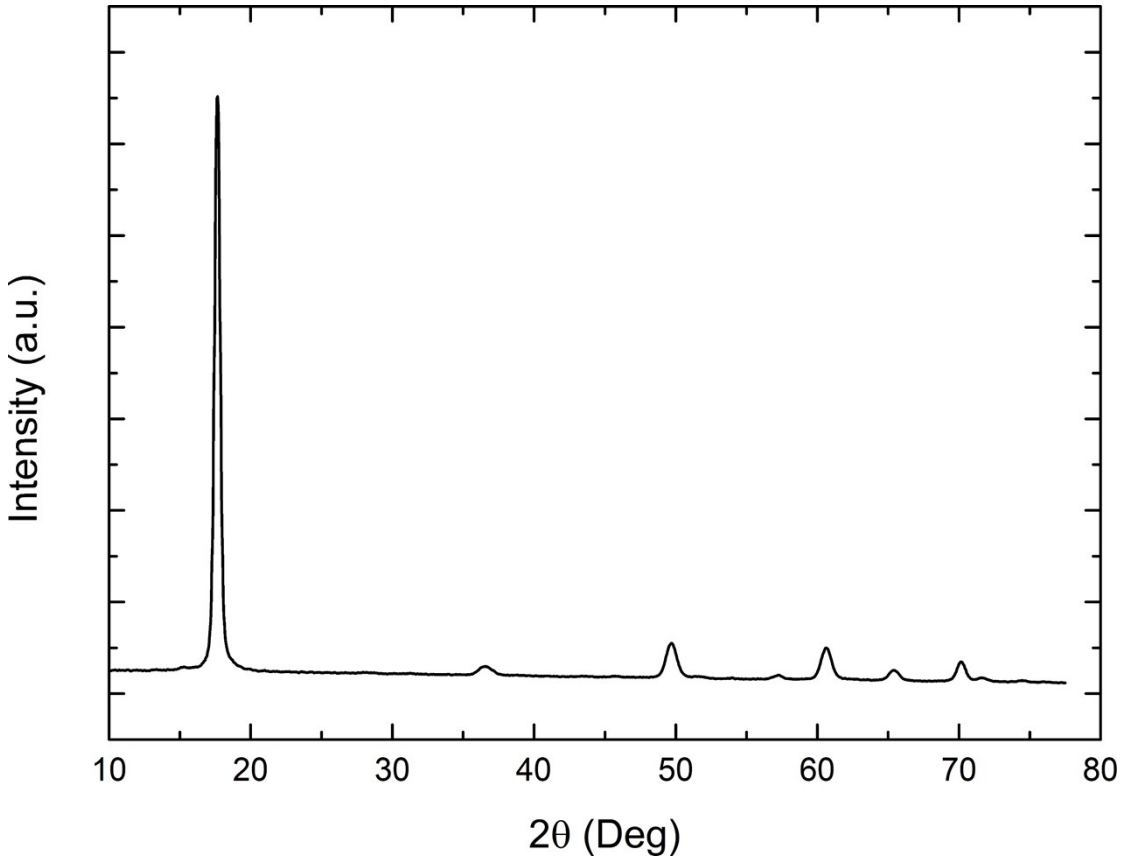

Fig S1. P-XRD of PyPbI3.

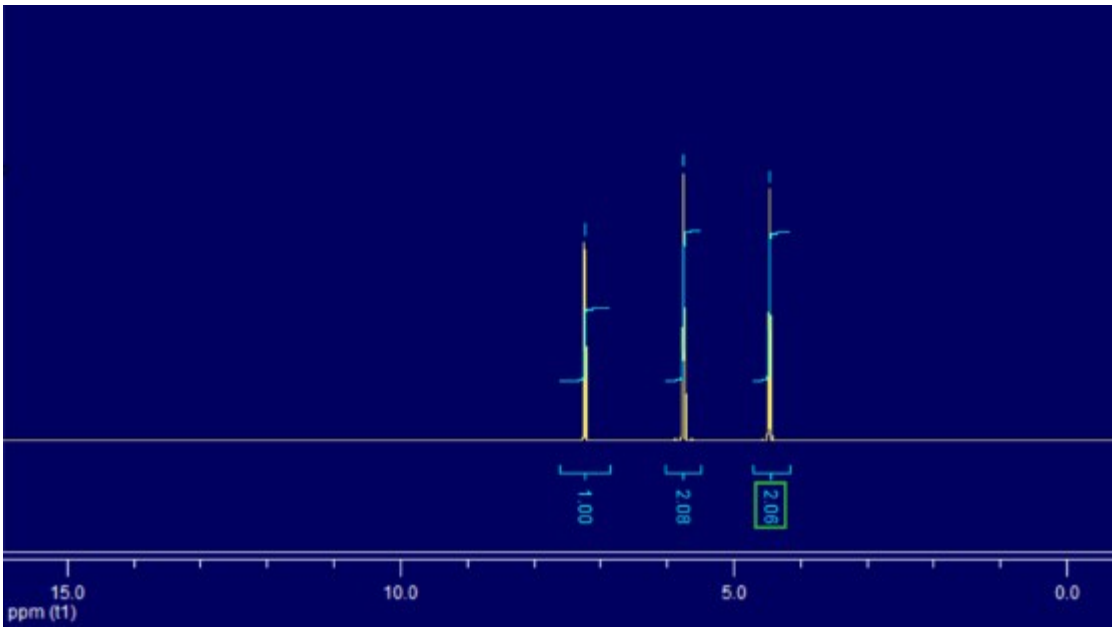

Fig S2. H-NMR result of the $PyPbI_3$ product.

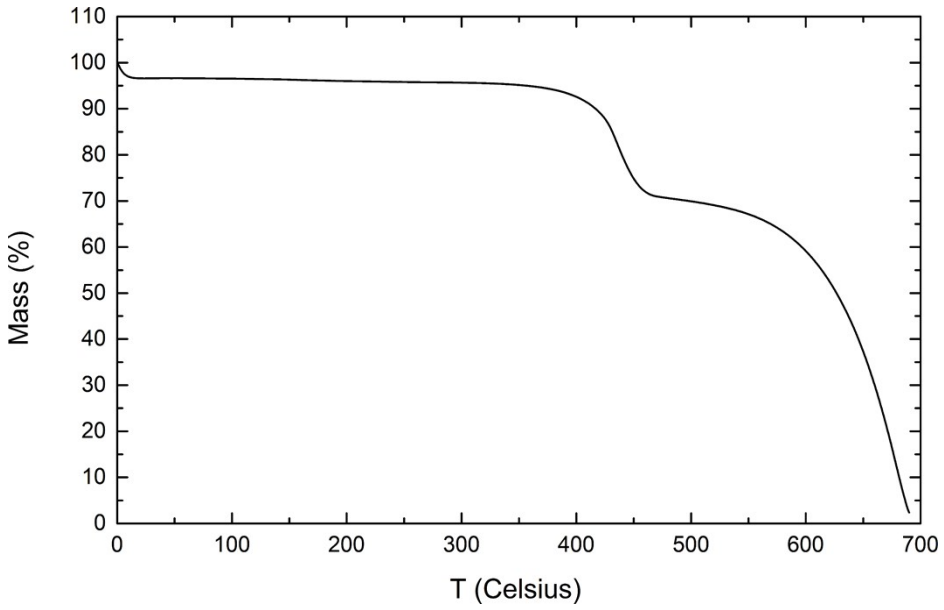

Fig S3. TGA curve of $PyPbI_3$. the product started weight dropping at 218°C, which indicates the original structure of $PyPbI_3$ remains stable even beyond 200°C. This is much higher than the phase transformation temperature of $MAPbI_3$, which is only around 55°C[9]. The weight loss then continues throughout the rest of the curve till 600 °C, where the $PyPbI_3$ decomposes completely.

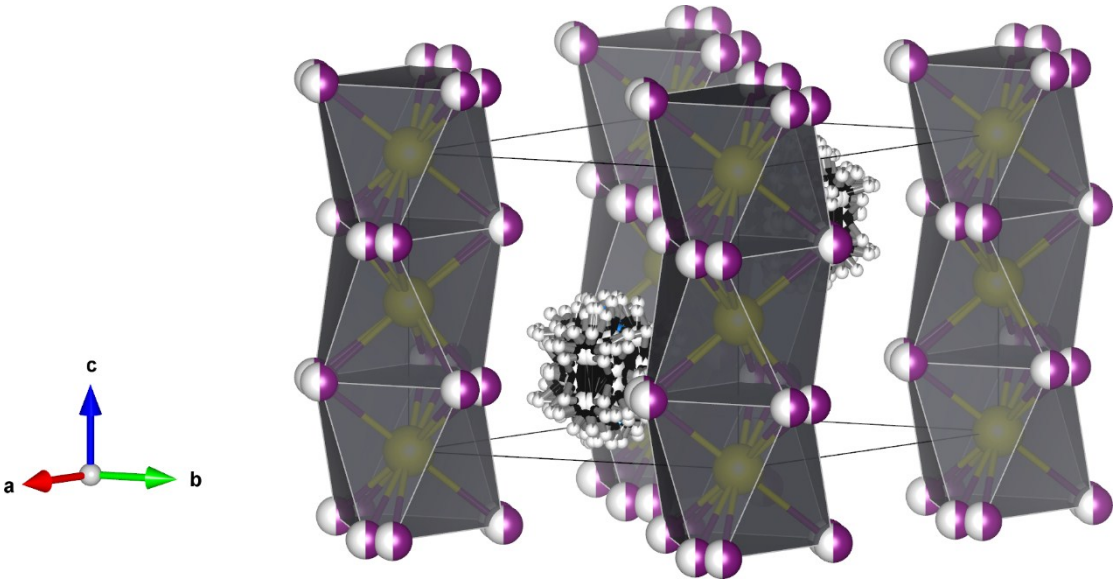

Fig S4. Crystal structure of $(C_4H_8NH_2)PbI_3$; lead yellow, iodine purple, carbon black, nitrogen blue and hydrogen grey. Reprinted with permission from ref. 26.

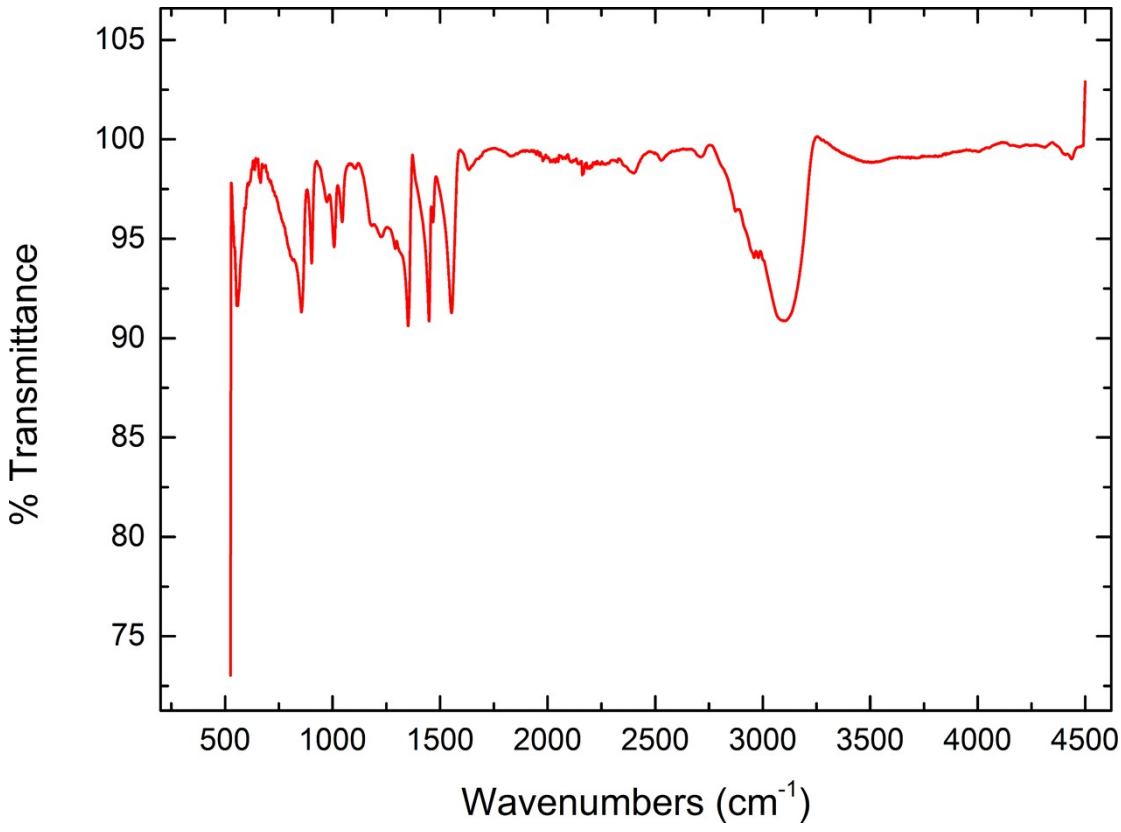

Fig S5. The FTIR spectra of the $PyPbI_3$ thin film. No sharp bands appear at $\mu < 840$ cm^{-1} or $\mu > 3500$ cm^{-1}, which means there is no water exist in the material. This is not surprising, considering that the $PyPbI_3$ product was annealed at 120℃ to form the thin film. All the other bands in the spectra can be assigned unambiguously to the pyrrolidinium cations. Moreover, their broadness is a clear indication of their orientational disorder, which was also confirmed by our single crystal XRD results. Obviously, the vibrations of the Pb-I skeleton are not visible in the explored wavenumber range.