Supporting Information

Stabilizing Lead Halide Perovskites with Quaternary Ammonium Cations: The Case of Tetramethylammonium Lead Iodide

Andrea Ciccioli¹*, Riccardo Panetta¹, Alessio Luongo¹, Bruno Brunetti², Stefano Vecchio Ciprioti³*, Maria Luisa Mele⁴, Alessandro Latini¹*

¹ Dipartimento di Chimica, Sapienza Università di Roma, Piazzale Aldo Moro 5, 00185 Roma, Italy
² Consiglio Nazionale delle Ricerche - Istituto per lo Studio dei Materiali Nanostrutturati, c/o Dipartimento di Chimica, Sapienza Università di Roma, Piazzale Aldo Moro 5, 00185 Roma, Italy
³ Dipartimento S.B.A.I, Sapienza Università di Roma, Via del Castro Laurenziano 7, 00161 Roma, Italy

⁴ Dipartimento I.C.M.A., Sapienza Università di Roma, Via Eudossiana 18, 00184 Roma, Italy

*corresponding authors.



Fig. S1. X-ray powder diffraction pattern of N(CH₃)₄PbI₃ after isothermal treatment at 295 °C for 10 hours.



Fig. S2. X-ray powder diffraction pattern of $N(CH_3)_4PbI_3$ after isothermal treatment at 298 °C for 10 hours.



Fig. S3. X-ray powder diffraction pattern of $N(CH_3)_4PbI_3$ after isothermal treatment at 300 °C for 10 hours.



Fig. S4. X-ray powder diffraction pattern of N(CH₃)₄PbI₃ after isothermal treatment at 302 °C for 10 hours.



Fig. S5. X-ray powder diffraction pattern of $N(CH_3)_4PbI_3$ after isothermal treatment at 305 °C for 10 hours.



Fig. S6. X-ray powder diffraction pattern of N(CH₃)₄PbI₃ acquired with environmental chamber at 127 °C.



Fig. S7. TG-DTA curves of $N(CH_3)_4PbI_3$ acquired in combination with QMS-EGA. The point of maximum ion currents intensities due to the gases evolved by the sample is indicated by an arrow.



Fig. S8. Quadrupole mass spectrum of the carrier gas (Ar) used in the TG-DTA/QMS-EGA experiment.



Fig. S9. Mass spectrum acquired in correspondence of the maximum ion currents due to evolved gases in the TG-DTA/QMS-EGA experiment.

T/K	pTMA/Pa	pCH ₃ I/Pa	pTMA/pCH ₃ I	ln K*
474.0	0.00066	0.00066	1.00	-37.673
458.0	8.8e-05	0.00012	0.73	-41.396
486.0	0.0016	0.0020	0.82	-35.697
447.1	2.5e-05	2.9e-05	0.85	-44.054
461.8	0.00013	0.00015	0.88	-40.830
448.7	4.0e-05	3.7e-05	1.07	-43.346
435.7	1.0e-05	1.0e-05	1.04	-45.966
474.1	0.00033	0.00045	0.73	-38.742
456.8	6.6e-05	8.2e-05	0.81	-42.065
483.1	0.00094	0.0011	0.87	-36.824
434.3	4.5e-06	6.5e-06	0.70	-47.274
			Mean 0.86	

* The standard state is, as usual, the pure ideal gas at 1 bar

Table S1. Partial pressures of $N(CH_3)_3$ (TMA) and CH_3I measured by KEMS experiments carried out on the $N(CH_3)_4PbI_3$ perovskite, the corresponding ratio and the equilibrium constant of process (7).