Materials Advances

SUPPORTING INFORMATION

Relative Water Stability of Powder vs Thin Films of Organic-Inorganic Halide Perovskites Including Durability of a Thin Film Bis(thiophenyl)-Pyrrole Lead Iodide

Abdul Basit Naveed,[a] Matthew C. Mulvehill,[a] Aftab Javaid,[a] Craig A. Grapperhaus,[b] and Joshua M. Spurgeon[a*]

Synthesis of 2TPOI

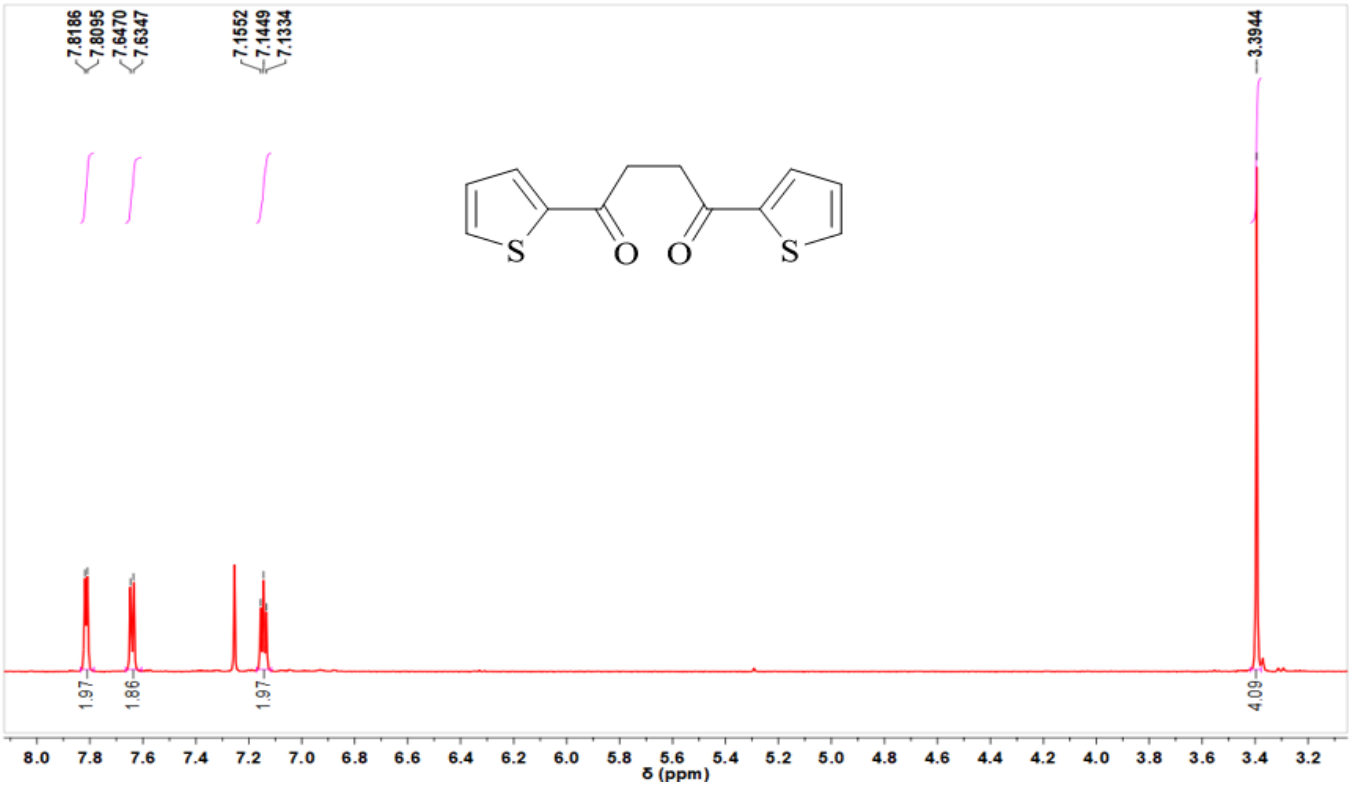

Fig. S1. ^{1}H-NMR spectra of 1,4-bis(2-thiophen-2-yl)butane-1,4-dione. (400 MHz $CDCl_3$) δ: 3.39 (t, 4H), 7.14 (t, 2H), 7.64 (d, 2H), 7.81 (d, 2H).

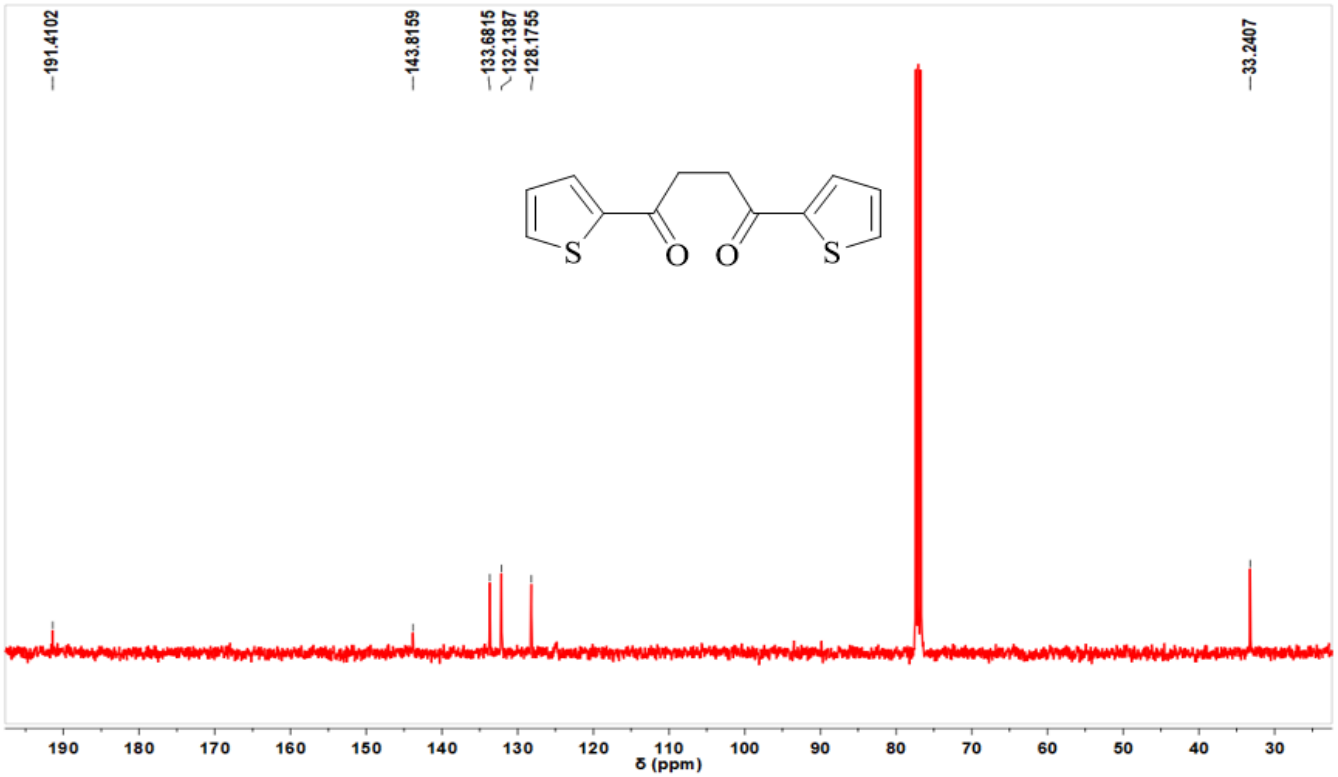

Fig. S2. ^{13}C-NMR spectra of 1,4-bis(2-thiophen-2-yl)butane-1,4-dione. (101 MHz $CDCl_3$) δ: 33.2, 128.17, 132.13, 133.68, 143.81, 191.41.

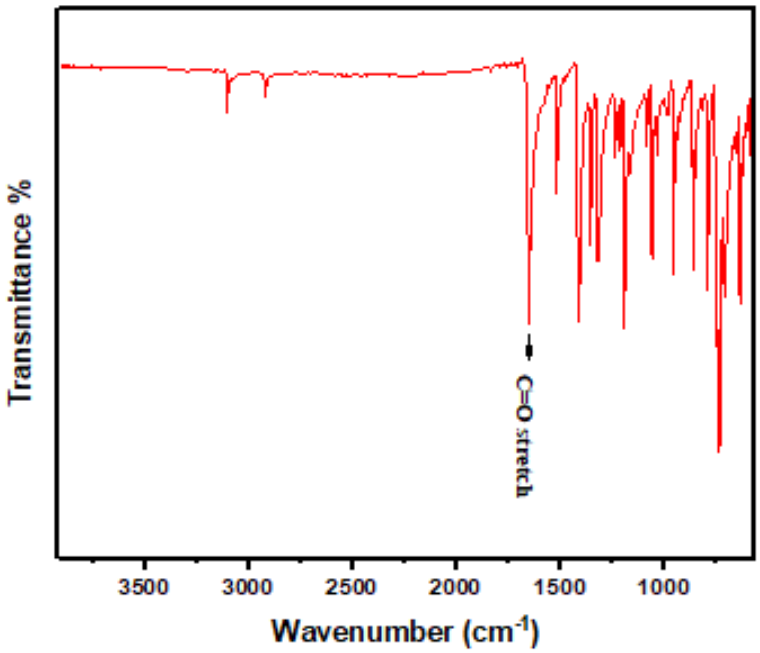

Fig. S3. FTIR spectra of 1,4-bis(2-thiophen-2-yl)butane-1,4-dione. 1647.63 cm^{-1} (C=O stretching vibration).

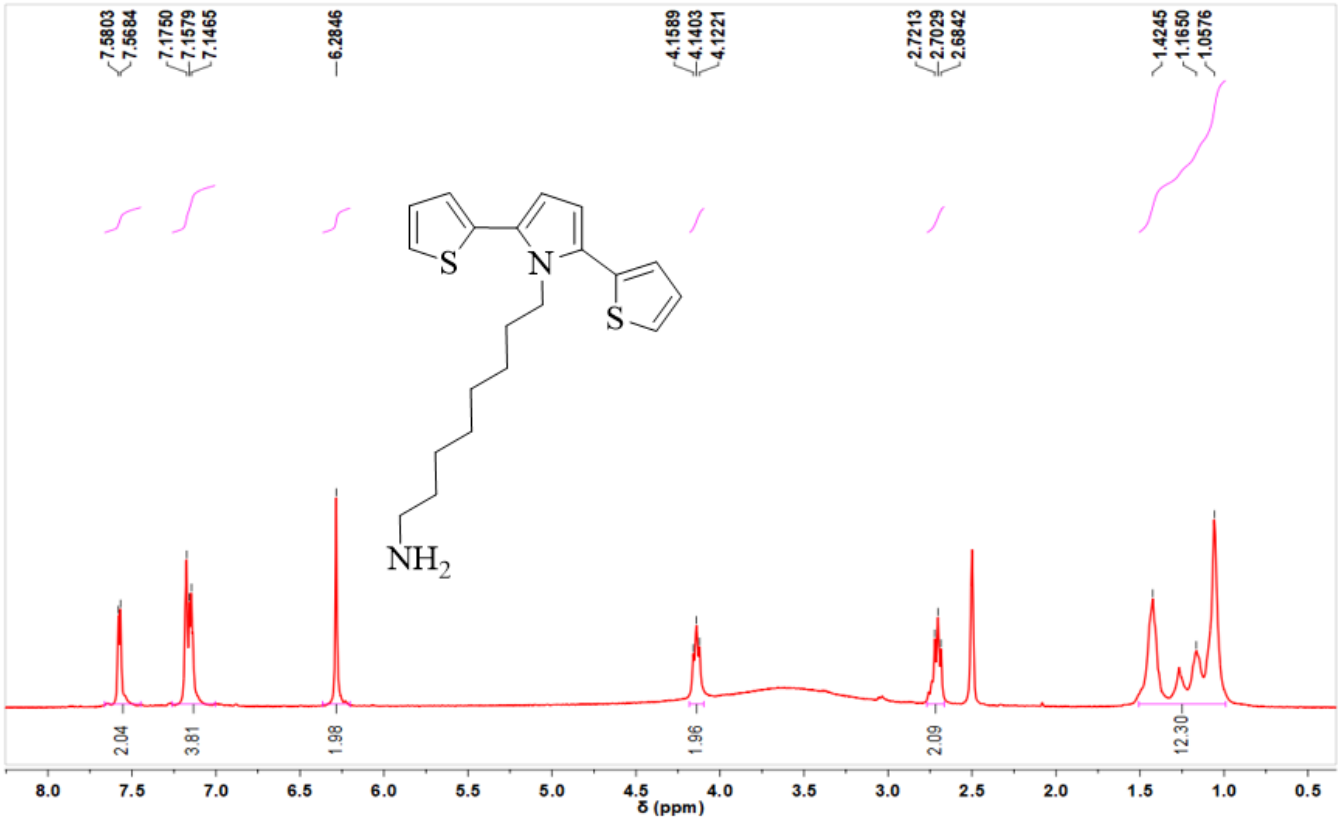

Fig. S4. ^{1}H-NMR spectra of 8-(2,5-bis(thiophen-2-yl)-1H-pyrrol-1-yl)-octylamine. (400 MHz DMSO-d_6) δ: 1.05-1.42 (m, 12H), 2.7 (t, 2H), 4.14 (t, 2H), 6.28 (s, 2H), 7.15 (m, 4H), 7.57 (d, 2H).

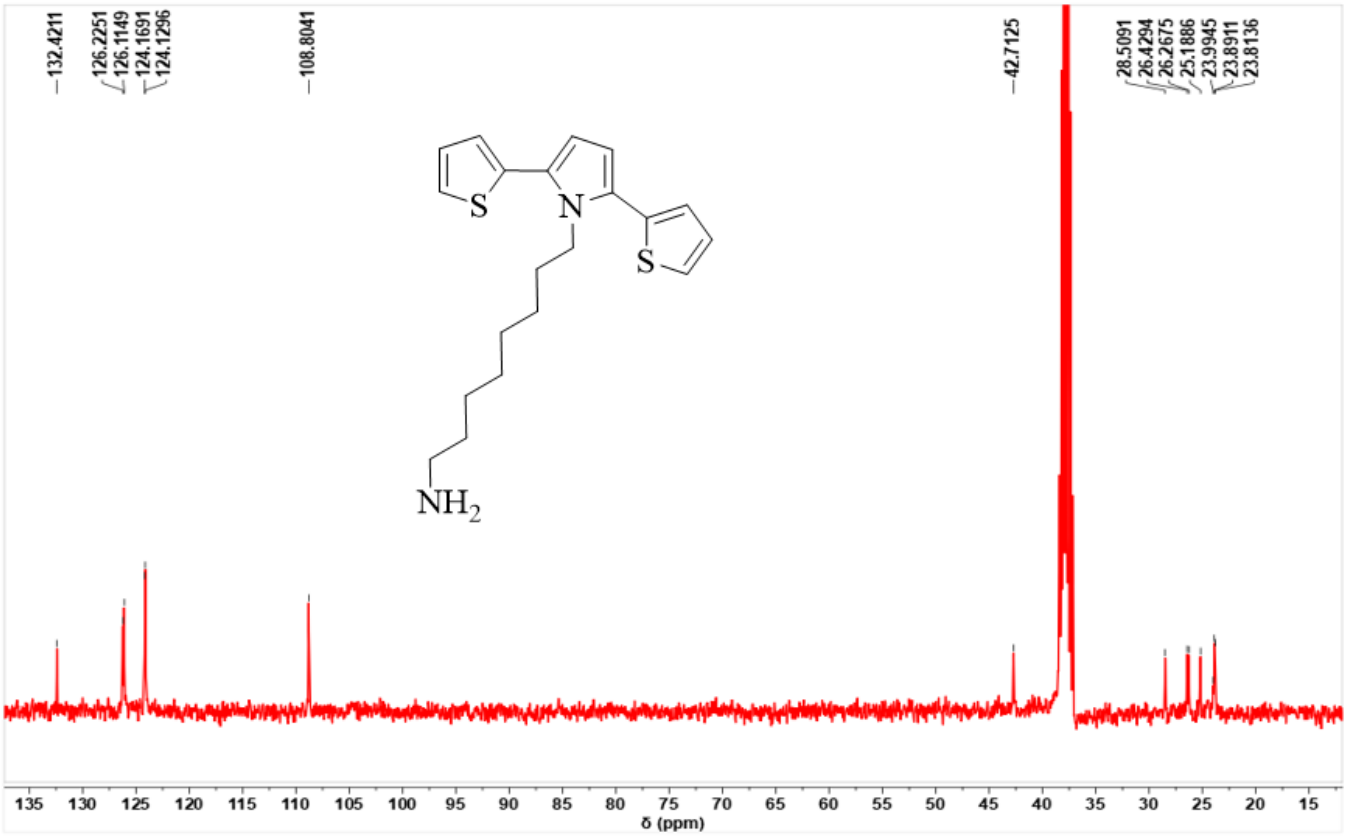

Fig. S5. ^{13}C-NMR spectra of 8-(2,5-bis(thiophen-2-yl)-1H-pyrrol-1-yl)-octylamine. (101 MHz DMSO-d_6) δ: 23.81, 23.89, 23.99, 25.18, 26.26, 26.42, 28.50, 42.71, 108.80, 124.12, 124.16, 126.11, 126.22, 132.42.

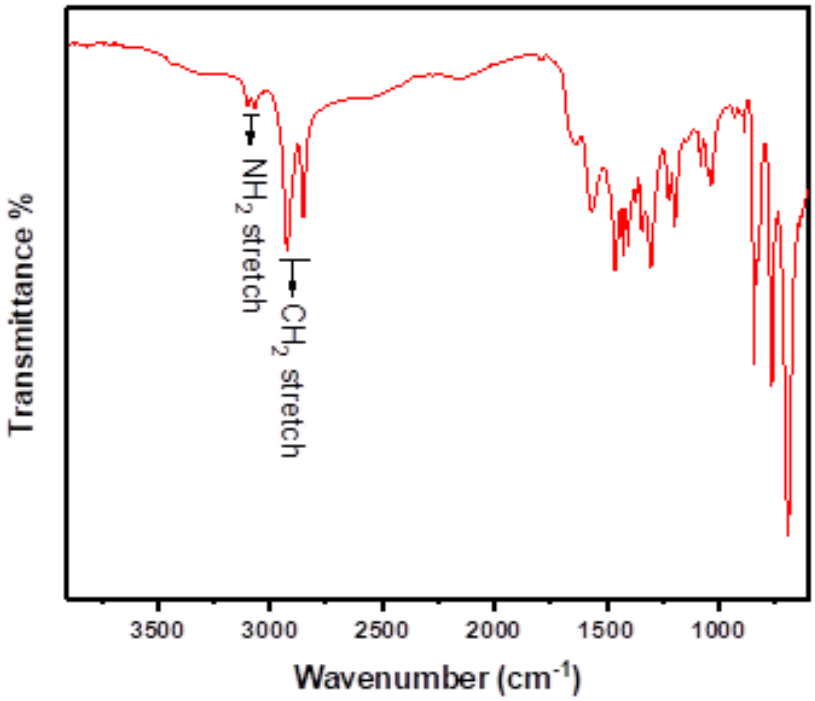

Fig. S6. FTIR spectra of 8-(2,5-bis(thiophen-2-yl)-1H-pyrrol-1-yl)-octylamine. 3064.33 cm^{-1} and 3102.90 cm^{-1} (-NH_2 stretching vibrations).

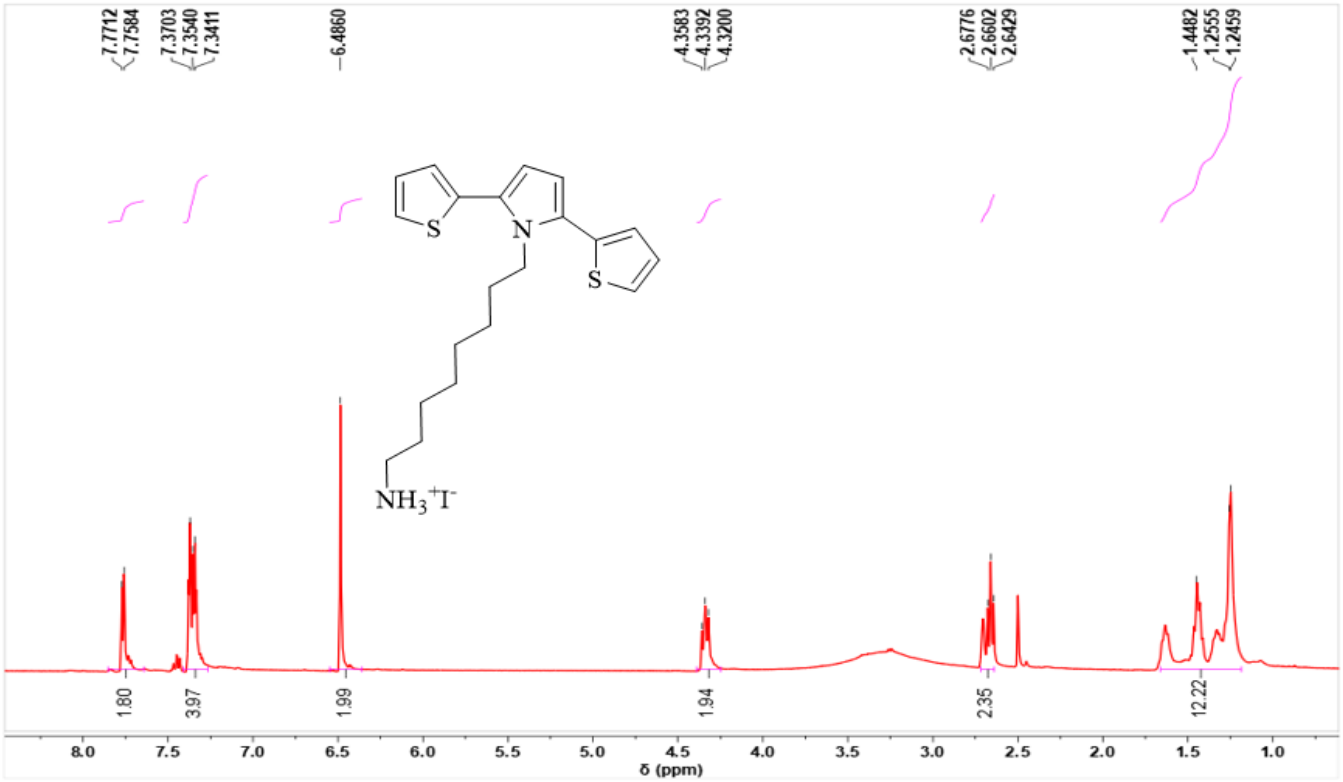

Fig. S7. ^{1}H-NMR spectra of 8-(2,5-bis(thiophen-2-yl)-1H-pyrrol-1-yl)-octylammonium iodide. (400 MHz DMSO-d_6) δ: 1.24-1.44 (m, 12H), 2.6 (t, 2H), 3.24 (t, 3H), 4.33 (t, 2H), 6.48 (s, 2H), 7.35 (m, 4H), 7.76 (d, 2H).

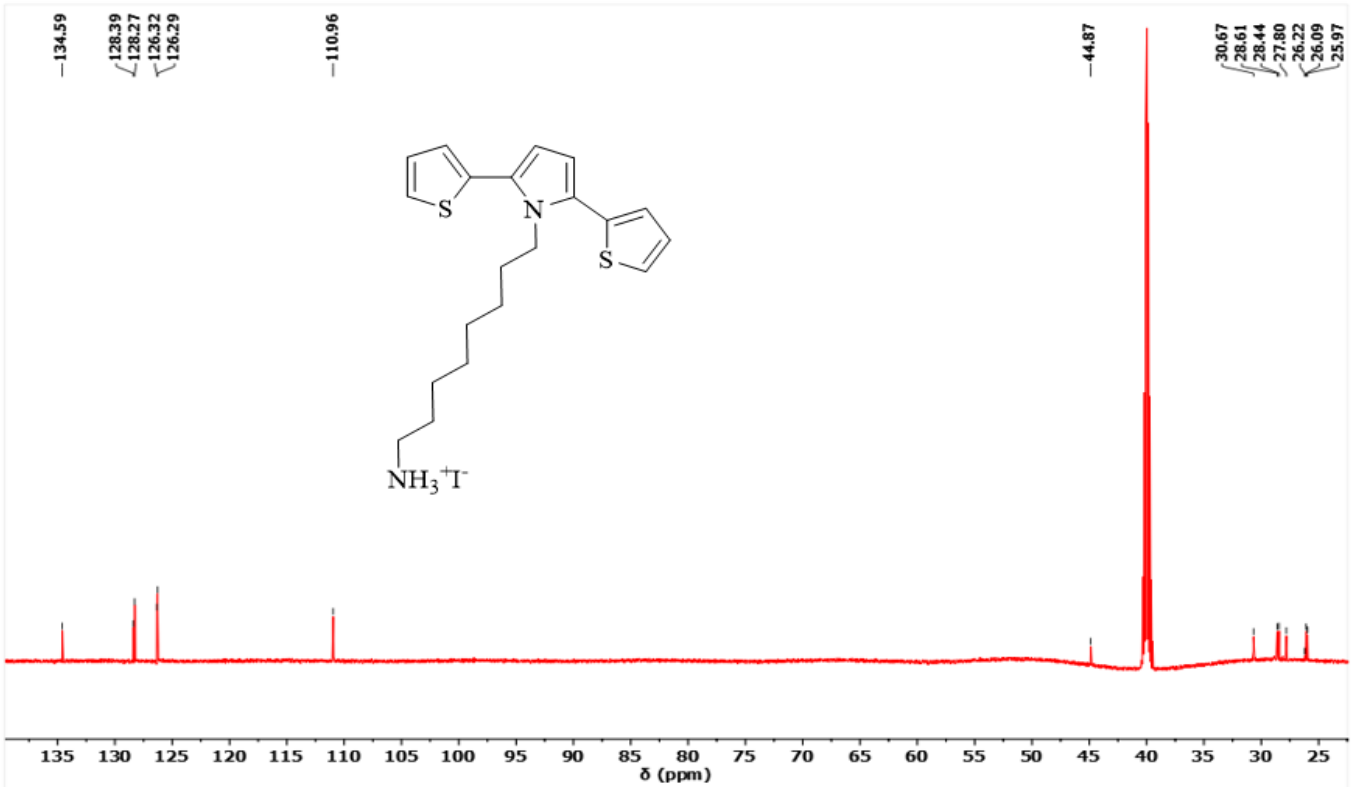

Fig. S8. ^{13}C-NMR spectra of 8-(2,5-bis(thiophen-2-yl)-1H-pyrrol-1-yl)-octylammonium iodide. (101 MHz DMSO-d_6) δ: 25.97, 26.09, 26.22, 27.80, 28.44, 28.61, 30.67, 44.87, 110.96, 126.29, 126.32, 128.27, 128.39, 134.59.

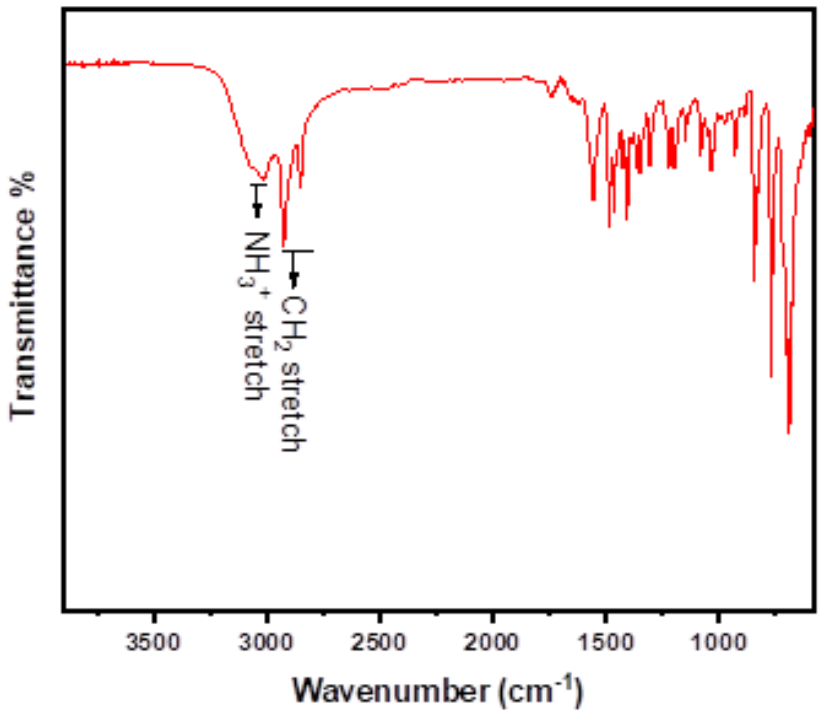

Fig. S9. FTIR spectra of 8-(2,5-bis(thiophen-2-yl)-1H-pyrrol-1-yl)-octylammonium iodide. Broad 2965-3090 cm^{-1} ($-NH_3^+$).

SEM/EDS of Microparticulate Powders

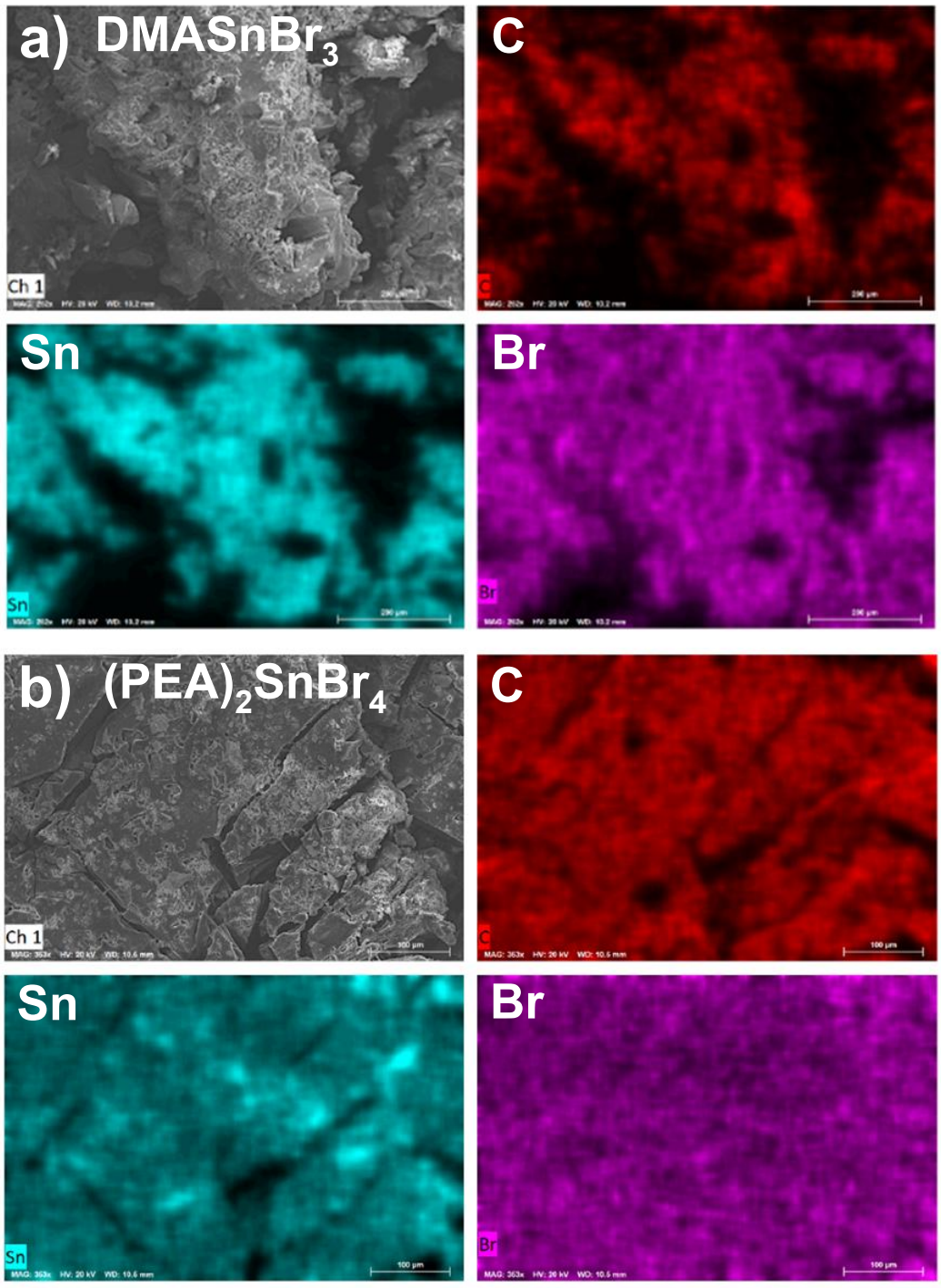

Fig. S10. SEM images (gray) and corresponding EDS elemental maps for C (red), Sn (blue), and Br (magenta) for powders of (a) $DMASnBr_3$ or (b) $(PEA)_2SnBr_4$.

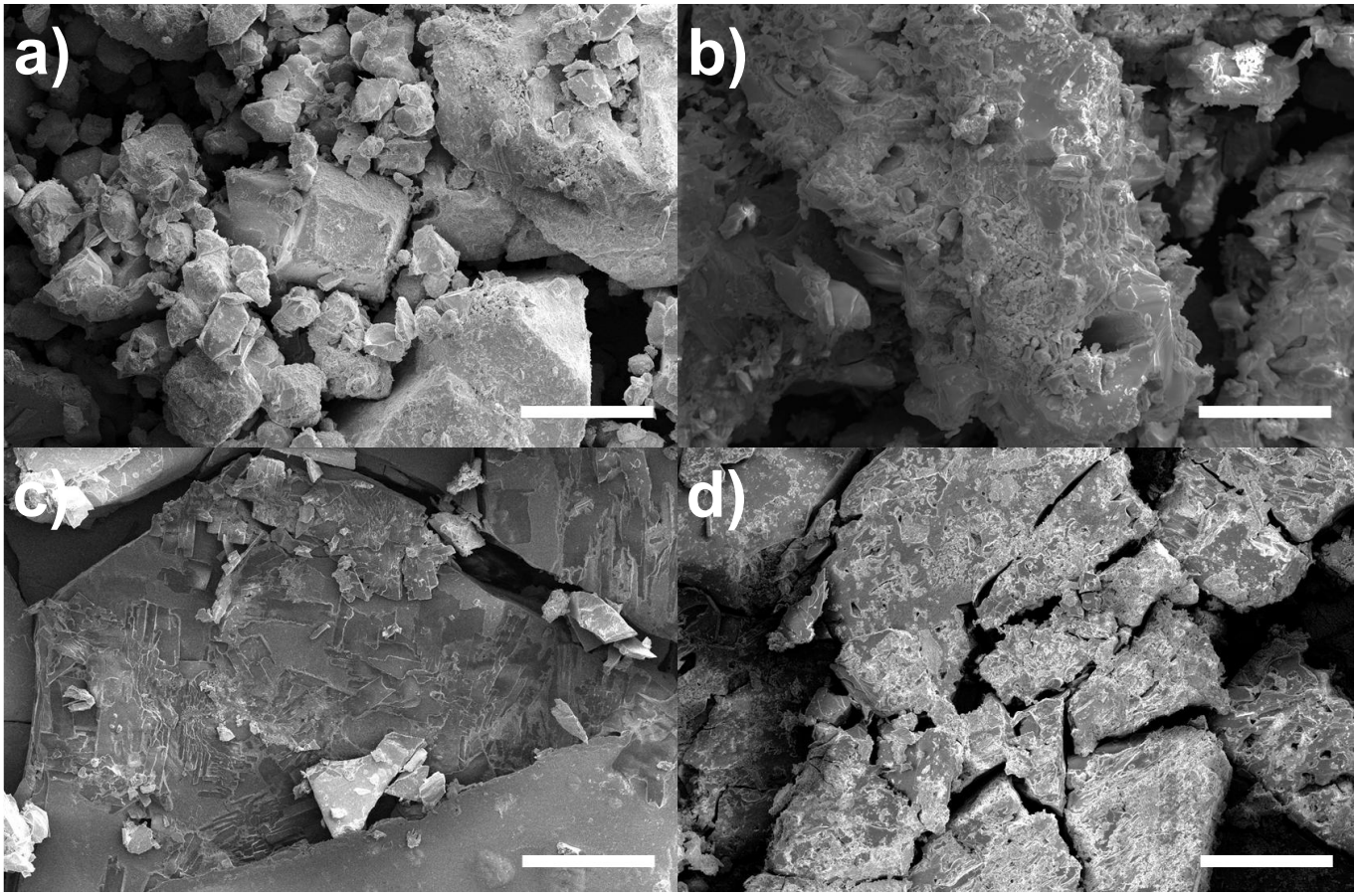

Fig. S11. SEM images of (a, b) $DMASnBr_3$ and (c, d) $(PEA)_2SnBr_4$ powders taken (a, c) before and (b, d) after stirring in water for 2 h. The samples images after water exposure are from the settled precipitate. The scale bar is 100 µm.

Surface Analysis

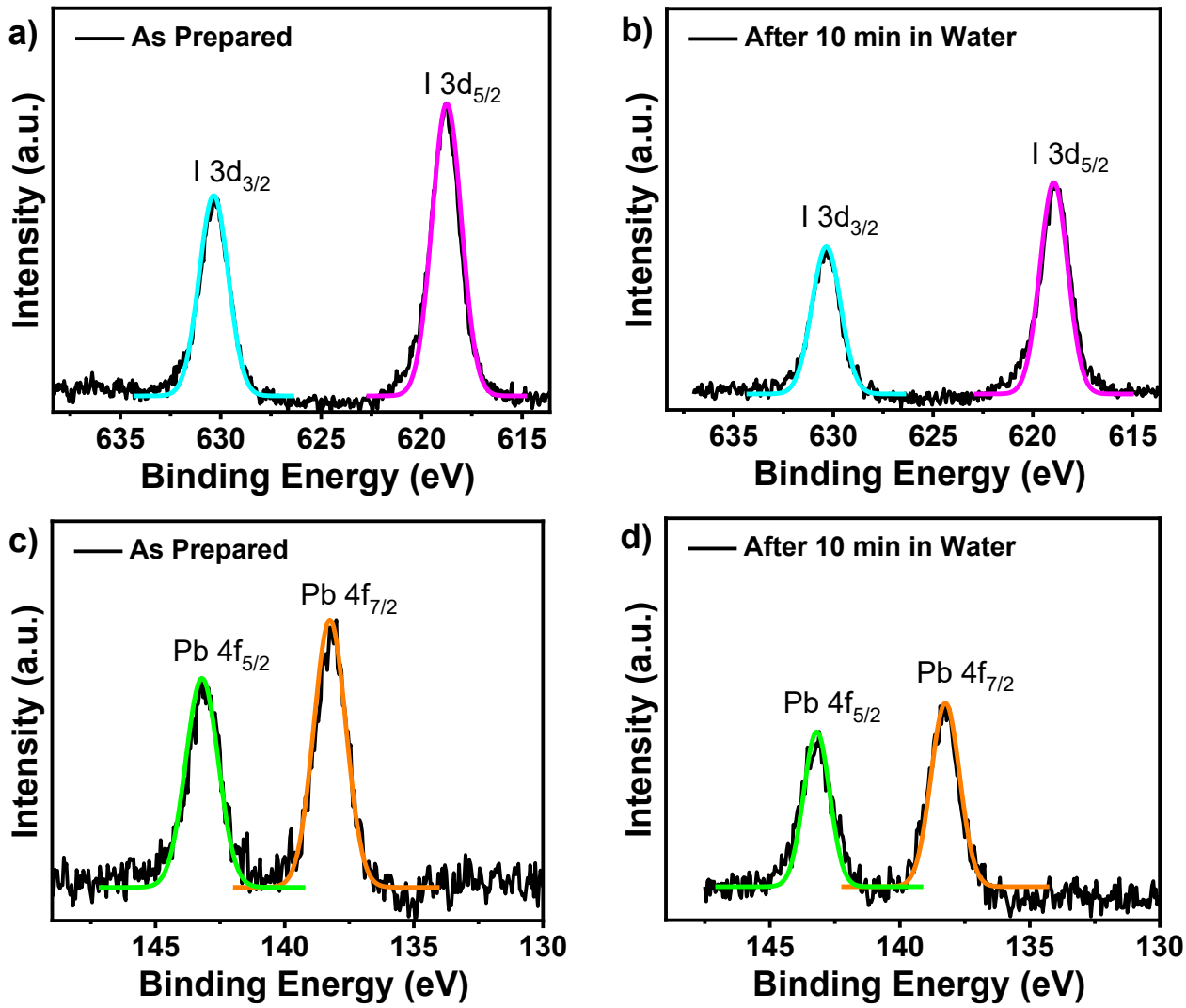

Fig. S12. XPS spectra with peak fittings of the (a-b) I 3d and (c-d) Pb 4f regions for thin films of $(2TPO)_2PbI_4$ perovskite (a, c) before and (b, d) after 10 min immersed in water.

Table S1. Quantitative metrics for the XPS spectra of the I 3d and Pb 4f regions for thin films of $(2TPO)_2PbI_4$ perovskite before and after 10 min immersed in water. FWHM = full width at half maximum. The area ratio is given as the area of each peak relative to the total area for both peaks of either the I 3d or Pb 4f.

	As Prepared			After 10 min in Water		
	Peak Position [eV]	FWHM [eV]	Area Ratio [%]	Peak Position [eV]	FWHM [eV]	Area Ratio [%]
I $3d_{3/2}$	630.35	1.82	40.7	630.35	1.77	41.3
I $3d_{5/2}$	618.85	1.82	59.3	618.95	1.77	58.7
Pb $4f_{5/2}$	143.17	1.43	43.7	143.08	1.20	43.2
Pb $4f_{7/2}$	138.27	1.43	56.3	138.17	1.20	56.8