The effect of an organic cation on electronic, optical and luminescent properties of 1D piperidinium, pyridinium, and 3-hydroxypyridinium lead trihalides.

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Supplementary information

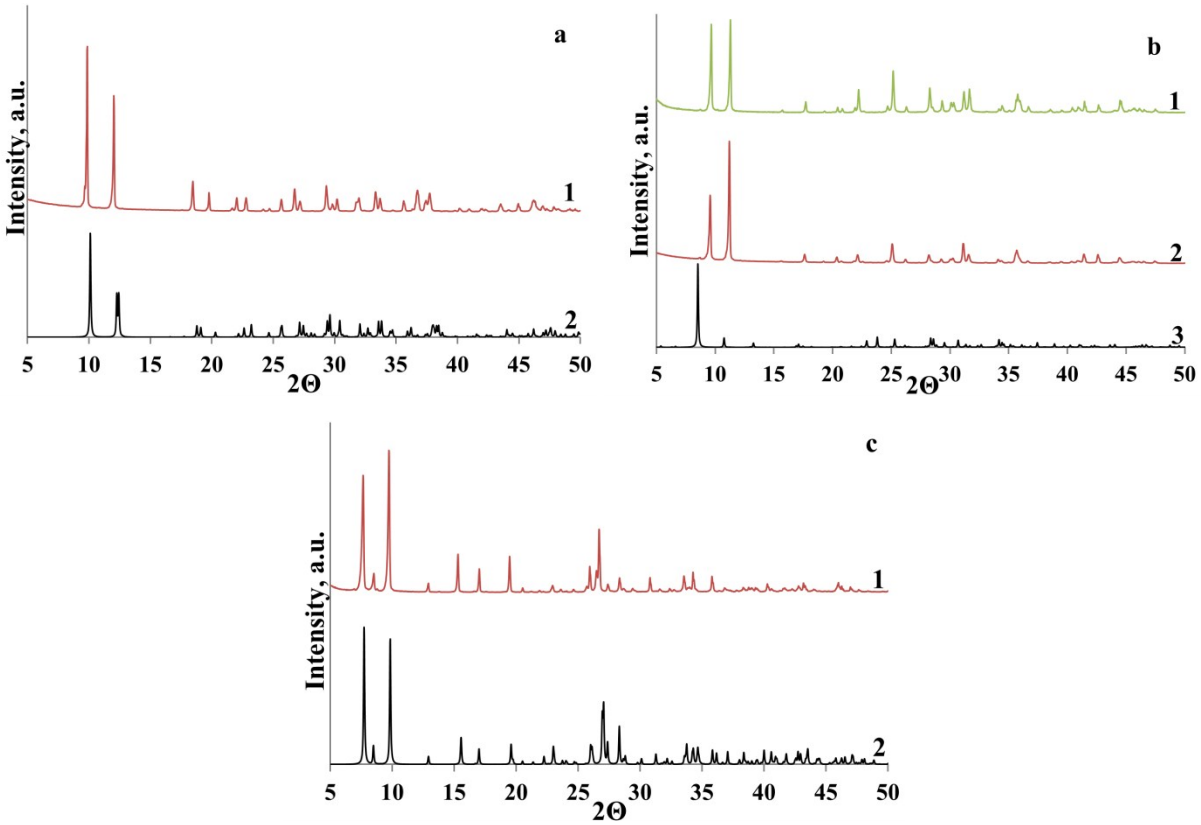

Figure S1. Experimental diffractograms of powdered $PipPbBr_3$ (a; curve 1), $PipPbI_3$ (b; curve 1), $2PipPbI_3 \cdot C_3H_7NO$ (b; curve 2), and 3-OH-$PyPbBr_3$ (c; curve 1) samples and their simulated counterparts (based on XRD analysis of single crystals) for $PipPbBr_3$ (a; curve 2), $PipPbI_3$ (b; curve 3), 3-OH-$PyPbBr_3$ (c; curve 2).

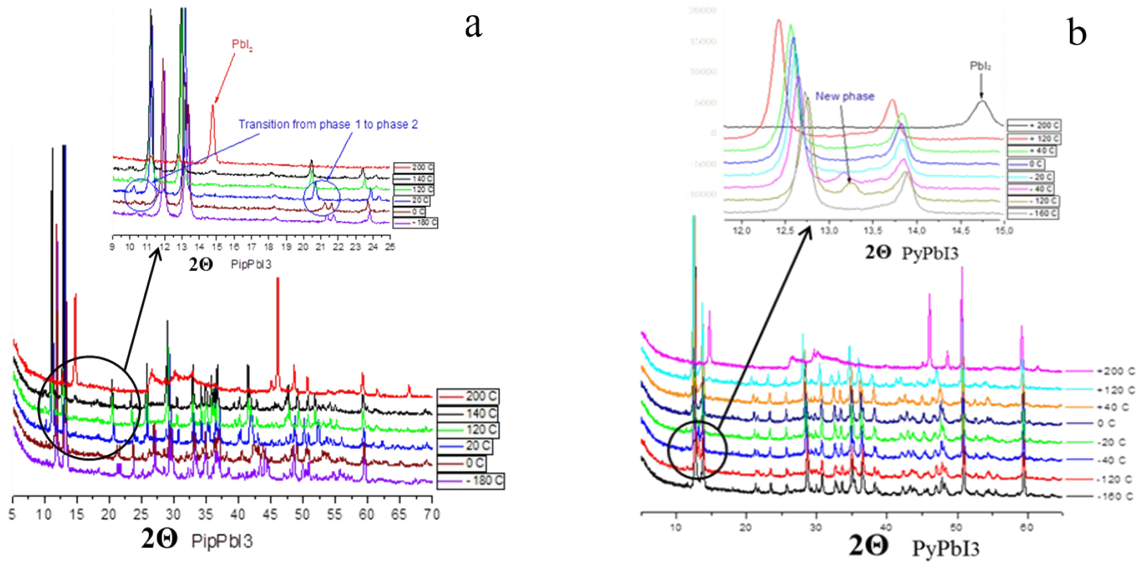

Figure S2. XRD data on $PipPbI_3$ (a) and $PyPbI_3$ (b) obtained at various temperatures.

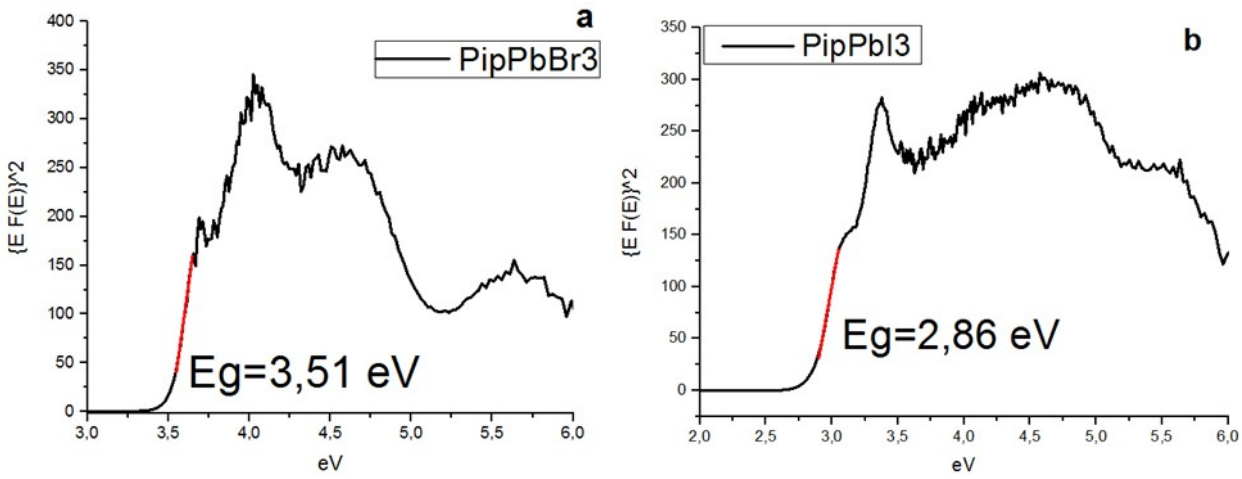

Figure S3. Tauc plots of diffuse reflectance spectra for $PipPbBr_3$ and $PipPbI_3$ in the case of direct (a, b) electronic transitions.

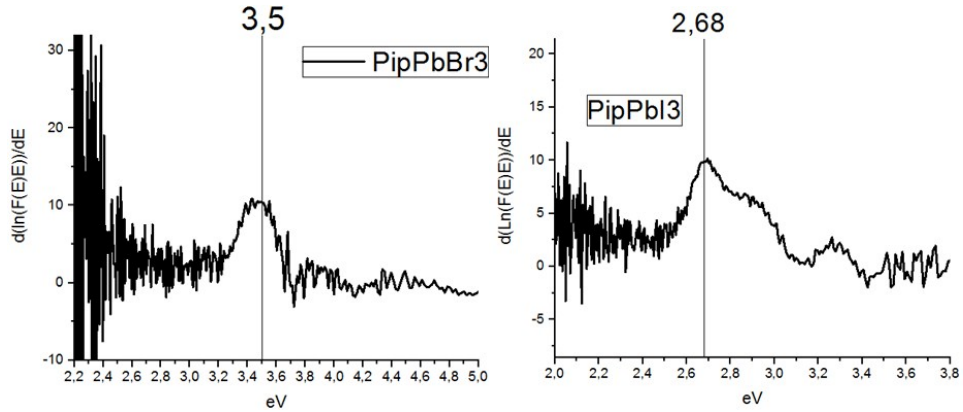

Figure S4. The dependence of lnF(E)E on E (eV) for $PipPbBr_3$ (left) and $PipPbI_3$ (right).

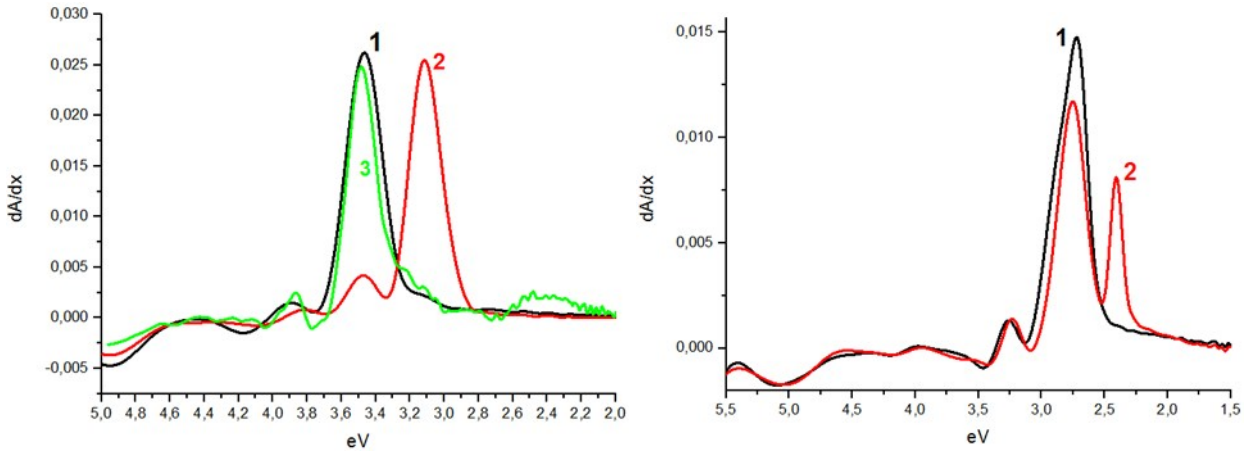

Figure S5. The dependence of a first derivative of absorption spectra on E (eV). Left: $PipPbBr_3$ (1), $PyPbBr_3$ (2), and 3-OH-$PyPbBr_3$ (3); right: $PipPbI_3$ (1) and $PyPbI_3$ (2).

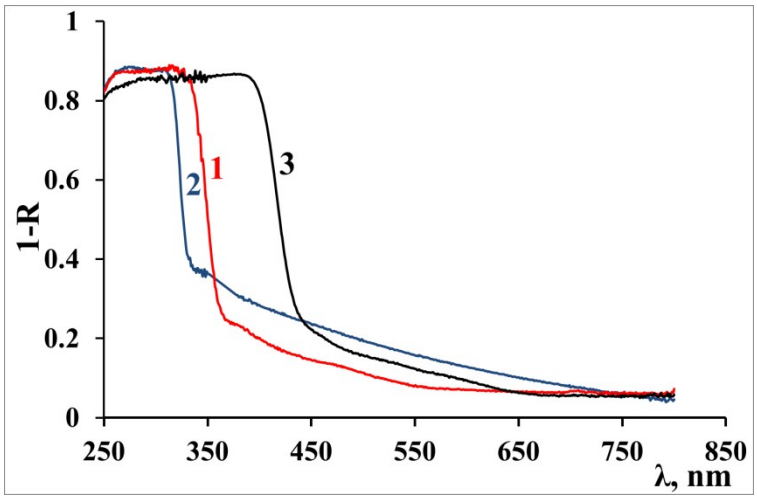

Figure S6. Absorption spectra of the salts: PyHBr (1), 3-OH-PyHBr (2), PyHI (3).

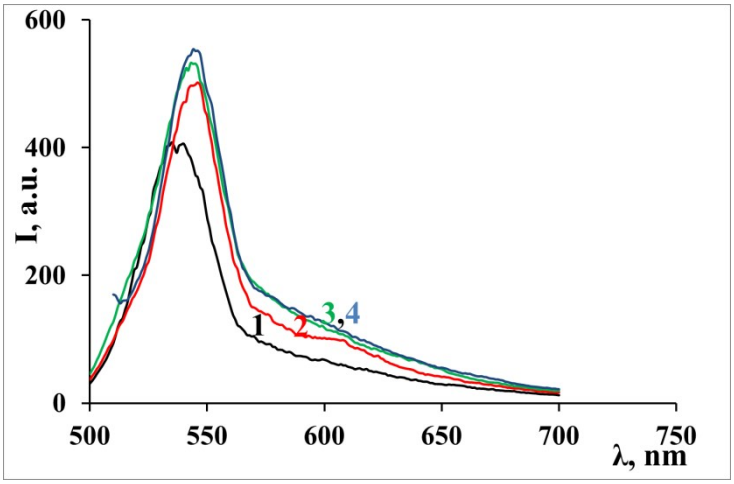

Figure S7. Luminescence spectra of 3-OH-$PyPbBr_3$ at $\lambda_{exc.}$: 390 nm (1), 450 nm (2), 470 nm (3), 490 nm (4).