Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Synthesis and investigation into structural, electronic and electrical properties of $K_2Pb(OCN)I_3$

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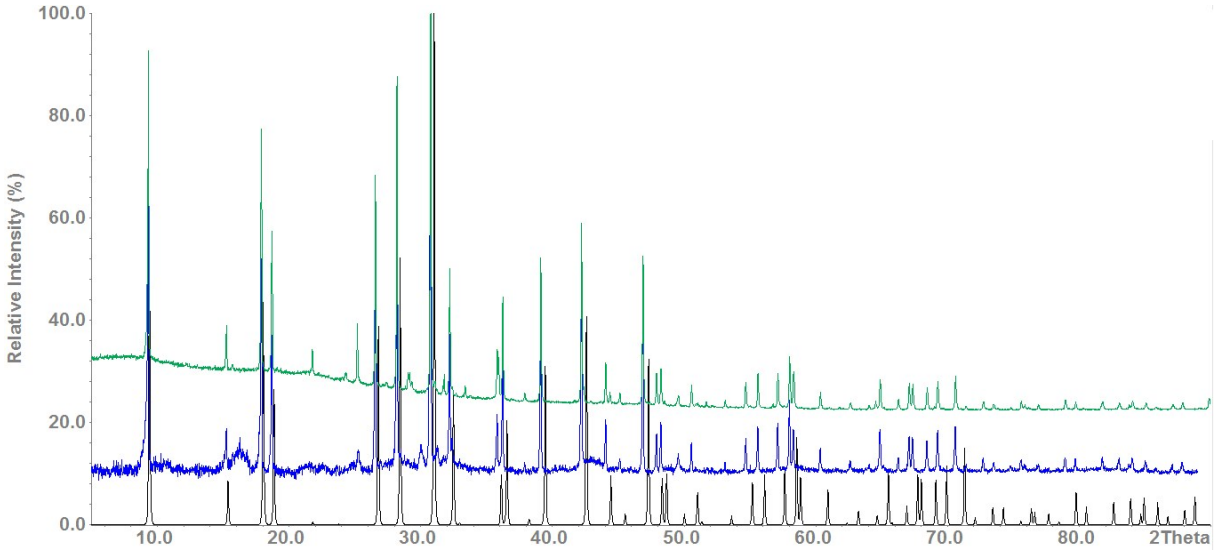

Figure S1. Powder X-ray diffraction patterns of the $K_2Pb(OCN)I_3$ compound. Theoretical pattern (black), the powder pattern resulting after sample heat treatment at 280 °C for 24 hours (blue) and 500°C for 15 hours (green). The powder patterns were collected with a Stadi-P (STOE, Darmstadt) powder diffractometer using germanium monochromator, a Cu-$K_{\alpha 1}$ source (λ=1.5406 Å) and a Mythen detector.

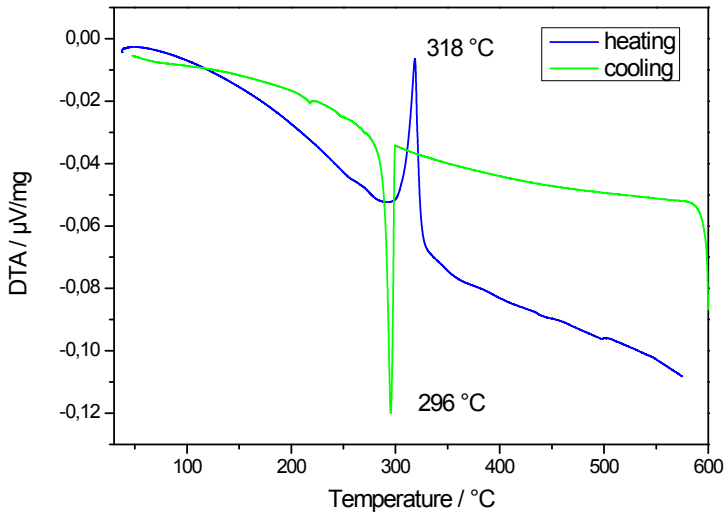

Figure S2. Second heating and cooling cycle examined by differential thermal analysis (DTA) of the reaction mixture of PbI_2+KOCN (1:1) performed under a flow of argon in a Netzsch Jupiter, STA 449 F3 apparatus, with about 100 mg of the reaction mixture being filled in an evacuated silica ampule.

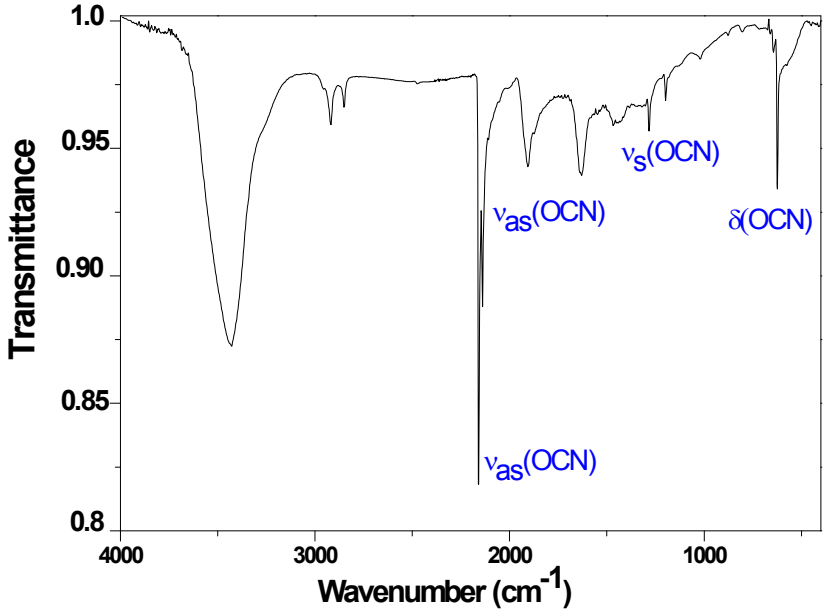

Figure S3. Fourier transform infrared spectrum of $K_2Pb(OCN)I_3$ compound.

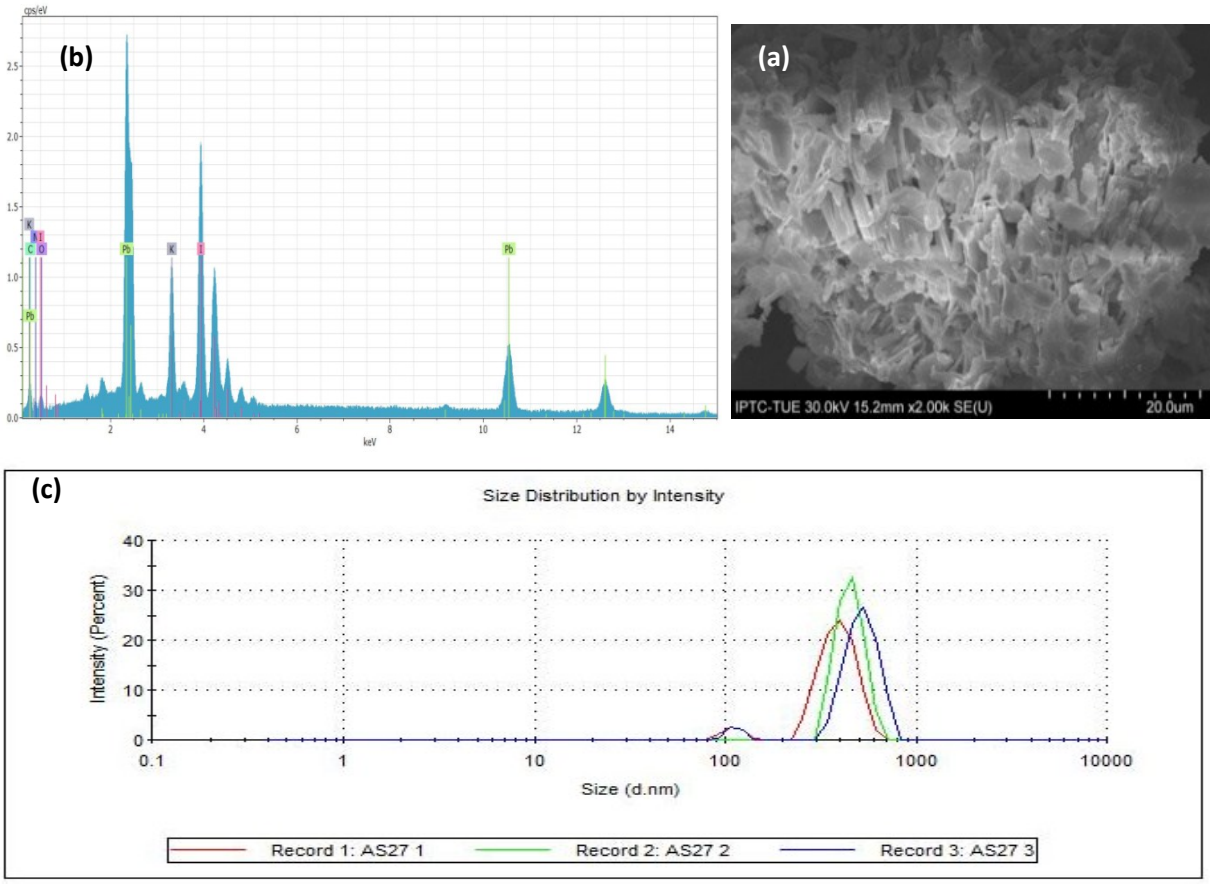

Figure S4. Scanning electron micrograph of a $K_2Pb(OCN)I_3$ pellet examined with the HITACHI SU8030 Scanning Electron Microscope (SEM) operated at 30 kV (a). EDX spectrum recorded at 30 kV (b), and dynamic light scattering (DLS) analysis of the $K_2Pb(OCN)I_3$ (c).

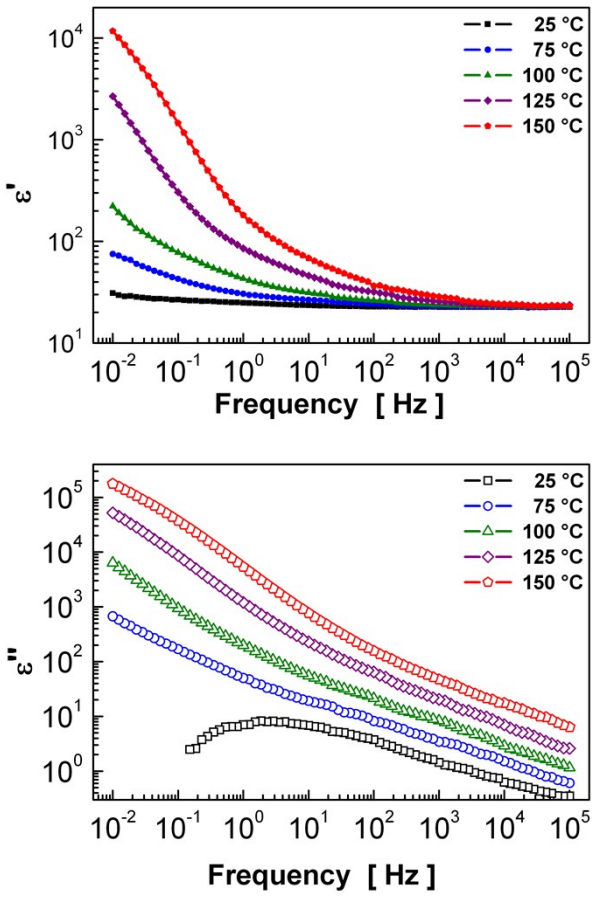

Figure S5. The frequency dependence of the complex permittivity at different temperatures. The values of the imaginary part of the permittivity (ε'') at 25 °C and frequencies below 10 Hz are affected by large errors and are only given as guideline. The downwards banding of the curve recorded at 25 °C is an artefact (the instrument is going out of the accurate measurement range).

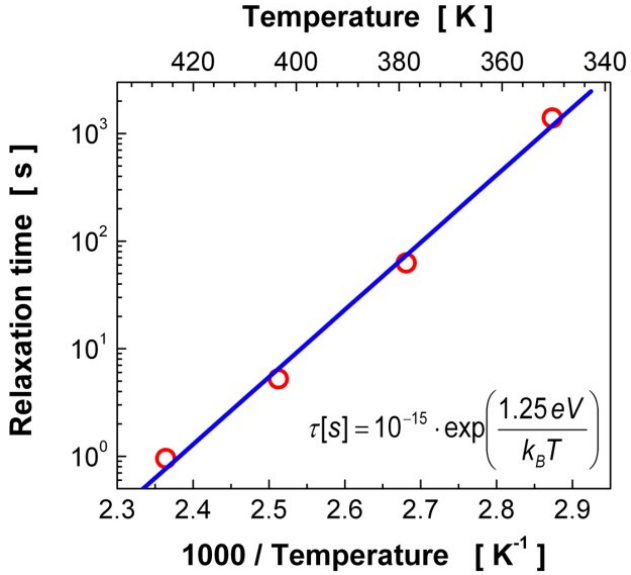

Figure S6. Dielectric relaxation time dependence on temperature. The impedance spectroscopy data have been fitted with ZView® software (Scribner&Associates).

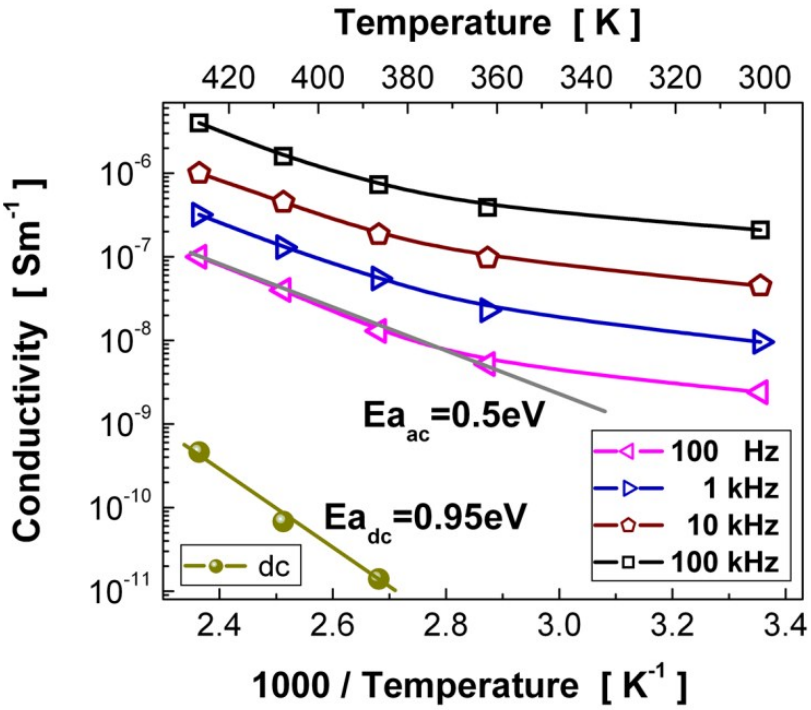

Figure S7. The temperature dependence of the dc and ac conductivity.

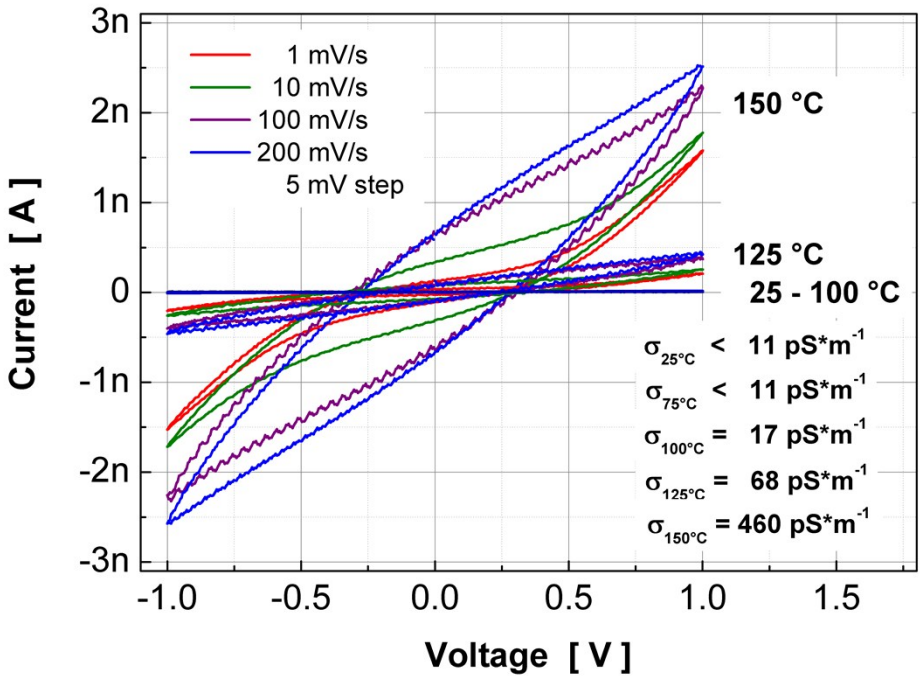

Figure S8. Cyclic current-voltage records at different temperatures. The average conductivities in the panel are calculated for a voltage range of 0.5 V (-250 to + 250 mV).