

(TMT-TTF)[Pb_{2.6/3}□_{0.4/3}I₂]₃: A TTF intercalated two-dimensional hybrid lead iodide: crystal structure and properties

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Figures

Fig. S1. The experimental powder XRD patterns and the simulated patterns from the crystal data of compounds (TMT-TTF)[Pb_{2.6/3}□_{0.4/3}I₂]₃ (**1**) and (TTF)Pb₂I₅.

Fig. S2. Thermogravimetric analysis of compound (TMT-TTF)[Pb_{2.6/3}□_{0.4/3}I₂]₃ (**1**).

Fig. S3. Asymmetric unit structure of compound (TMT-TTF)[Pb_{2.6/3}□_{0.4/3}I₂]₃ (**1**).

Fig. S4. Mott Schottky curves of (TTF)Pb₂I₅ coated electrodes.

Table

Table S1. Crystal data and structural refinement parameters for compound (TMT-TTF)[Pb_{2.6/3}□_{0.4/3}I₂]₃ (**1**).

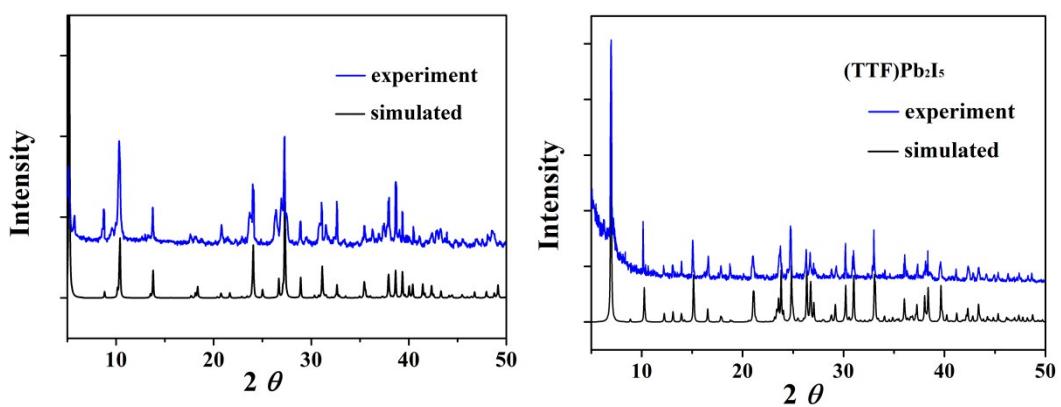


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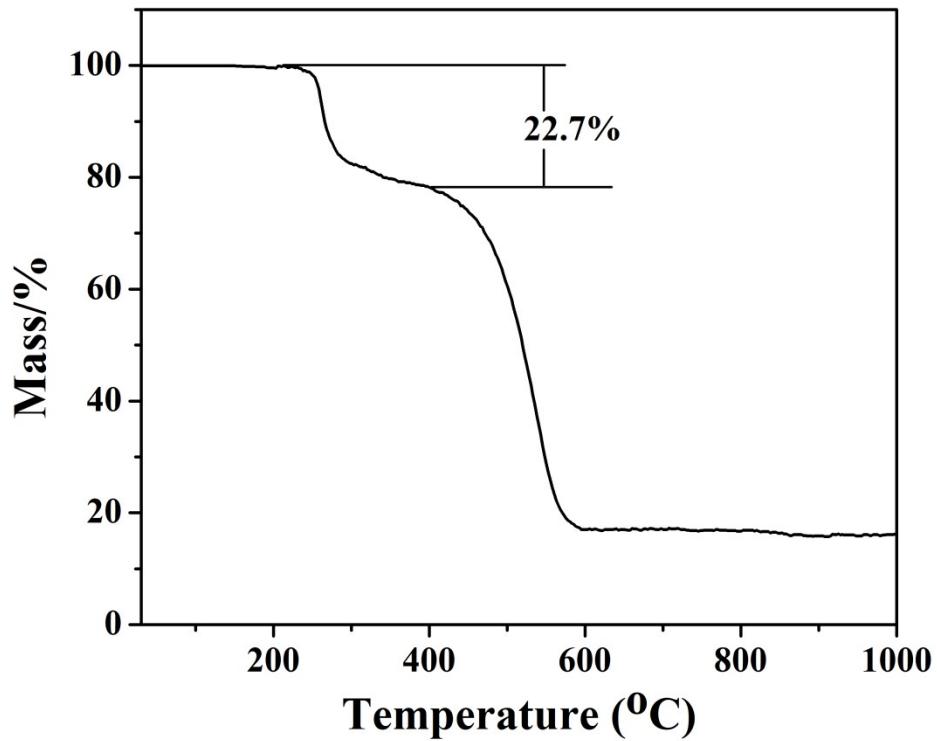


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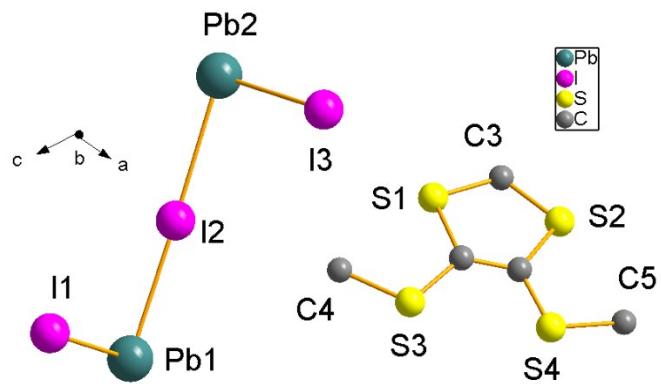


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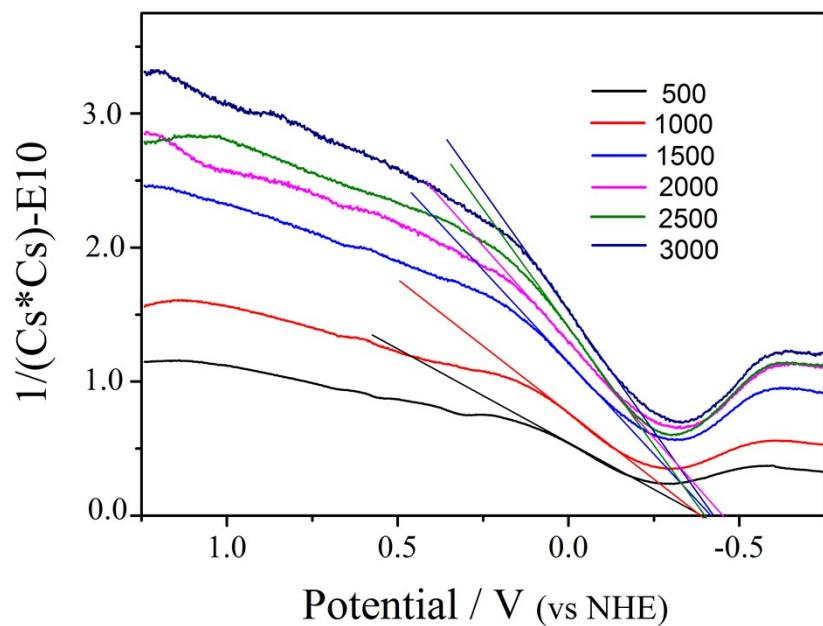


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formula	C ₁₀ H ₁₂ I ₆ Pb _{2.6} S ₈
fw	1688.77
cryst size (mm ³)	0.10×0.10×0.20
cryst syst	monoclinic
space group	<i>I</i> 2/ <i>m</i>
<i>a</i> (Å)	19.5549(14)
<i>b</i> (Å)	4.5007(2)
<i>c</i> (Å)	19.9119(9)
α (deg)	90
β (deg)	119.0050(14)
γ (deg)	90
<i>V</i> (Å ³)	1532.66(14)
Z	2
ρ_{calcd} (g cm ⁻³)	3.659
<i>F</i> (000)	1462
μ (mm ⁻¹)	20.839
<i>T</i> (K)	223(2)
reflns collected	24096
unique reflns	2003
observed reflns	1692
no. params	106
GOF on <i>F</i> ²	1.080
<i>R</i> ₁ [I>2σ(<i>I</i>)]	0.0305
<i>wR</i> ₂ [I>2σ(<i>I</i>)]	0.0544