Supporting Information for

Tetrathiafulvalene-based double metal lead iodides, structures and electrical properties

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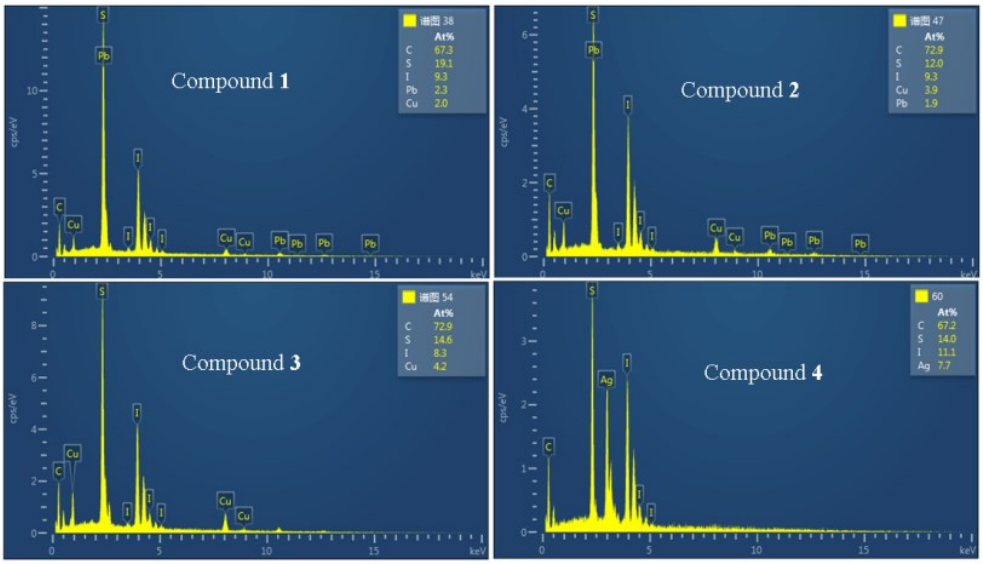

Fig. S1. EDX of compounds **1**–**4**, showing no existence of Cl element and verifying the Pb/Cu ratios of **1** (1:1) and **2** (1:2).

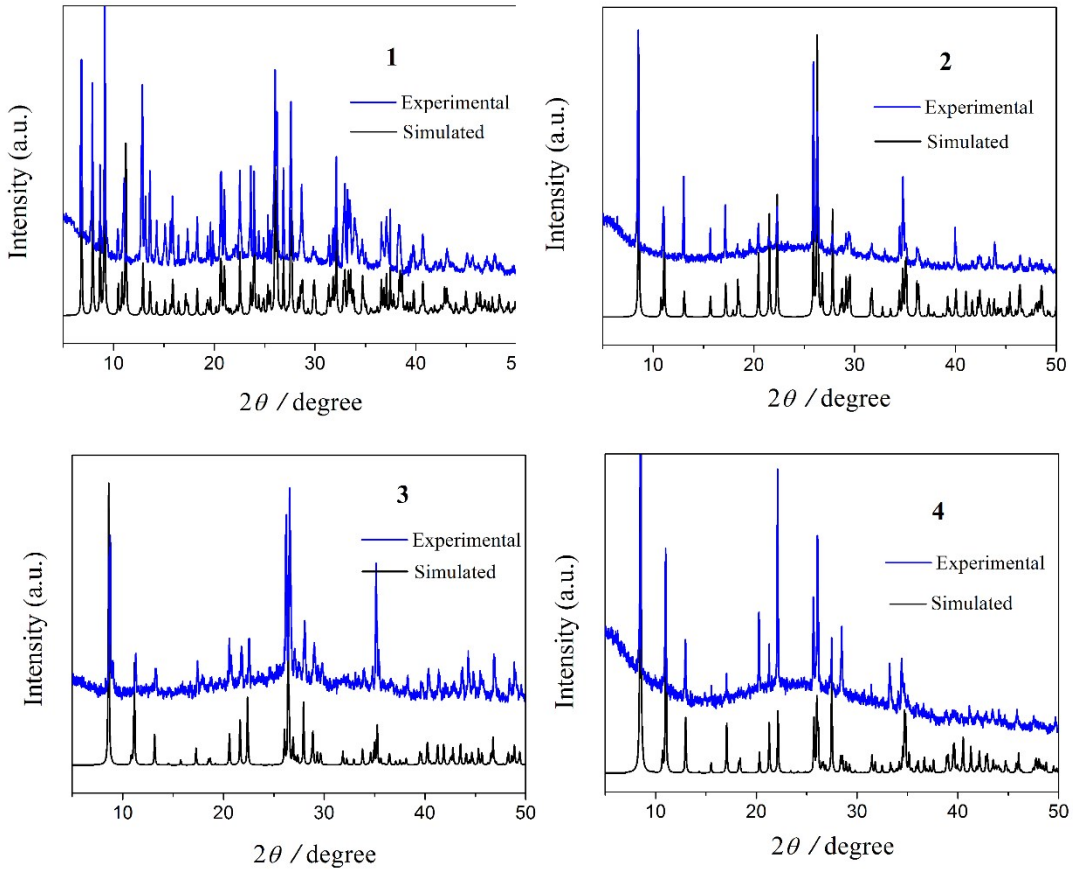

Fig. S2. The experimental powder XRD pattern and the simulated pattern from the crystal data of compounds **1**–**4**.

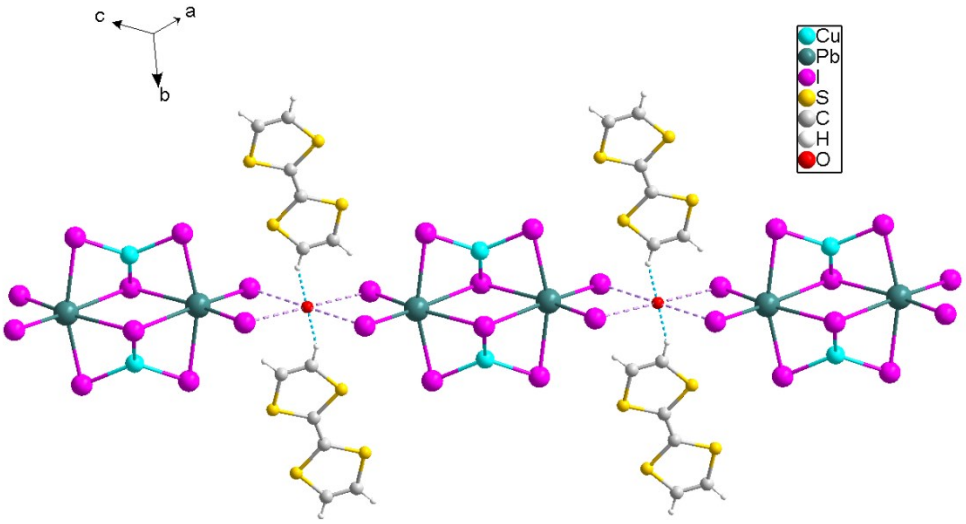

Fig. S3. Water molecule connects two neutral TTF with two anions through hydrogen bonds to be a 1D structure in **1**.

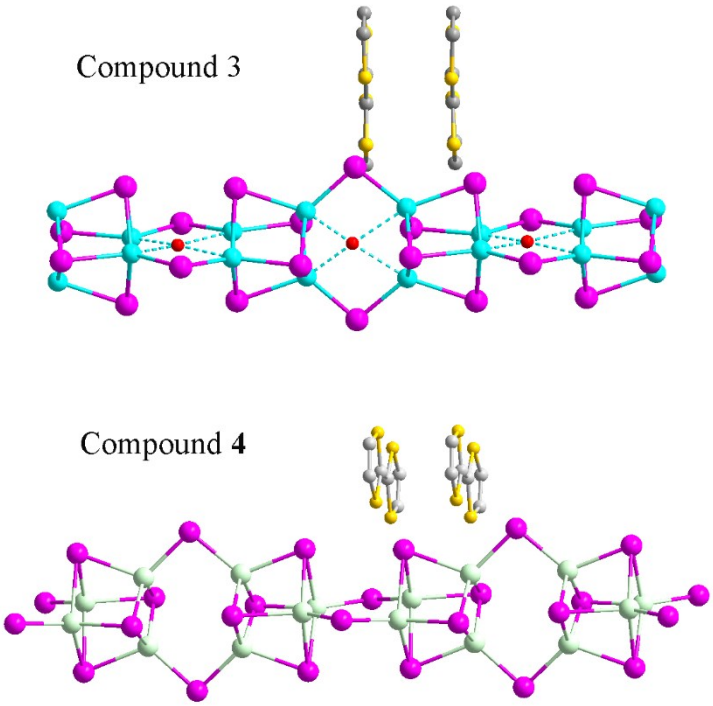

Fig. S4. Molecular structures of compounds **3** and **4**, showing the similarity in anion structure and different in co-crystallized water molecule.

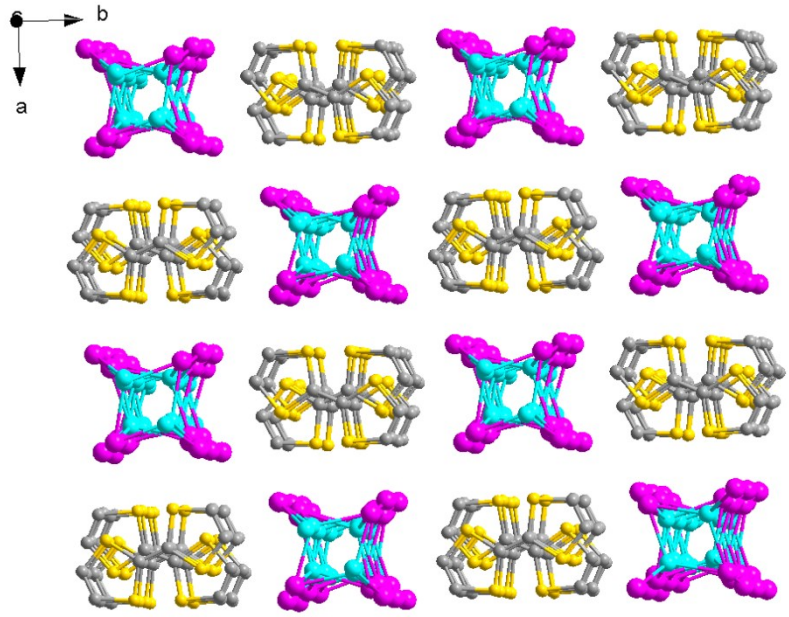

Fig. S5. Assembly of the cation columns and anion chains in compound **3** and **4**.

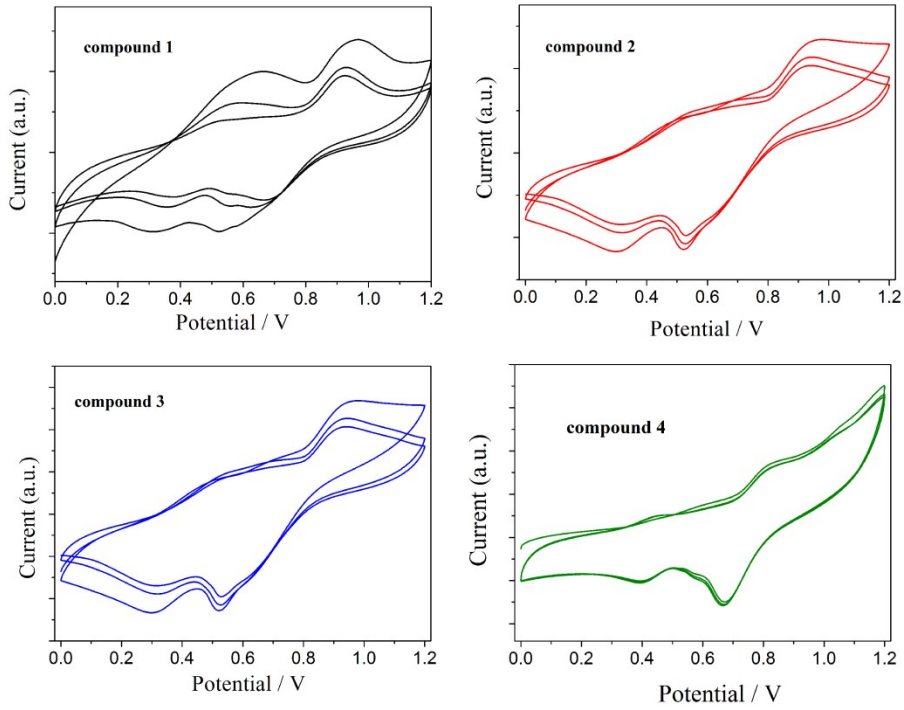

Fig. S6. Cyclic voltammograms of **1**–**4**, showing the multiple cycles (in solid state, at a scan rate of 100 mV s^{-1}, vs SCE, CH_3CN, Bt_4NClO_4).

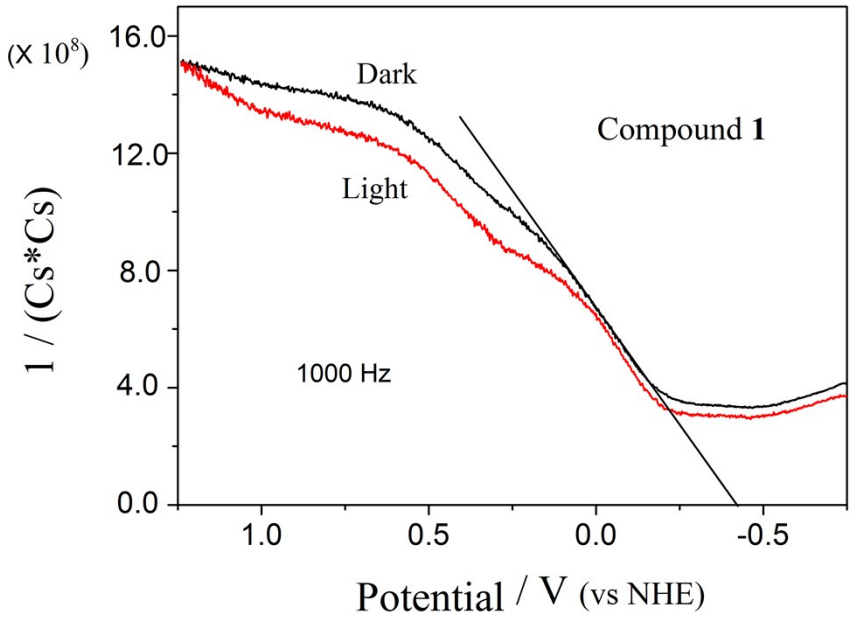

Fig. S7. Mott–Schottky plots of **1** measured in Na_2SO_4 solution.

Table S1. Crystal data and structural refinement parameters for compounds **1**–**4**.

	1	**2**	**3**	**4**
formula	$C_{30}H_{22}Cu_2I_{10}OPb_2S_{20}$	$C_{12}H_8Cu_2I_6PbS_8$	$C_{12}H_{10}Cu_4I_6OS_8$	$C_{12}H_8Ag_4I_6S_8$
Fw	2850.13	1504.33	1442.35	1601.62
cryst size (mm^3)	0.2×0.08×0.08	0.2×0.2×0.1	0.3×0.2×0.1	0.4×0.2×0.1
cryst syst	triclinic	orthorhombic	orthorhombic	orthorhombic
space group	$P\bar{1}$	*Cccm*	*Pccn*	*Pccn*
a (Å)	10.9196(19)	15.931(4)	13.4453(16)	16.135(3)
b (Å)	11.281(2)	13.531(3)	15.8728(19)	13.700(2)
c (Å)	13.700(2)	13.491(3)	13.4449(16)	13.745(3)
α (deg)	86.986(4)	90	90	90
β (deg)	70.722(4)	90	90	90
γ (deg)	80.970(4)	90	90	90
V ($Å^3$)	1573.3(5)	2908.2(12)	2869.3(6)	3038.3(10)
Z	1	4	4	2
ρ_{calcd} (g cm^{-3})	3.006	3.436	3.334	3.501
F(000)	1282	2664	2600	2856
μ (mm^{-1})	11.60	14.172	9.972	9.192
T (K)	213(2)	213(2)	213(2)	213(2)
reflns collected	24275	6952	23502	26196
unique reflns	7015	1745	3196	3464
observed reflns	5679	1272	2564	2301
no. params	290	72	141	136
GOF on F^2	1.031	1.027	1.019	1.007
R_1[I>2σ(*I*)]	0.0466	0.0479	0.0353	0.0408
$_wR_2$[I>2σ(*I*)]	0.1222	0.1237	0.0901	0.0906

Table S2. Short C···C, S···S, C···S and S···I interaction in compounds **1**–**4**.

			C···C distance (Å)			
1	C3···C9	3.404(13)	C4···C6	3.385(13)	C10···C10	3.639(13)
2	C3···C3	3.303(12)	C3···C3	3.495 (12)		
3	C3···C6	3.324(8)				
4	C3···C6	3.402(8)				
			S···S distance (Å)			
1	S2···S6	3.435(3)	S3···S7	3.399(3)	S4···S8	3.420(3)
	S4···S9	3.527(5)				
2	S1···S1	3.319(3)	S2···S2	3.374(4)	S1···S1	3.650(3)
3	S1···S3	3.326(3)	S2···S4	3.356(2)	S1···S3	3.643(2)
4	S1···S3	3.376(3)	S2···S4	3.396(4)		
			S···C distance (Å)			
1	S2···C14	3.494(18)	S4···C15	3.278(11)	S4···C15	3.144(11)
2	-					
3	S3···C1	3.494(7)				
4	-					
			S···I distance (Å)			
1	S3···I1	3.767(4)	S6···I5	3.551(4)	S7···I3	3.633(3)
	S9···I2	3.768(3)	S10···I1	3.681(3)		
2	S2···I2	3.710(3)				
3	S2···I1	3.695(2)	S4···I1	3.703(2)		
4	S2···I1	3.772(3)				