Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

A New Antimony-Based Organic-Inorganic Hybrid Absorber with Photoconductive Response

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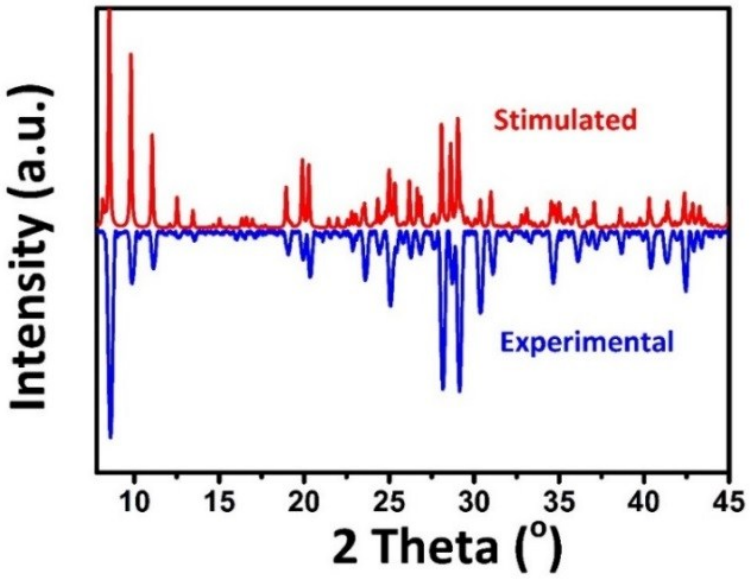

Figure S1. PXRD patterns of **1**.

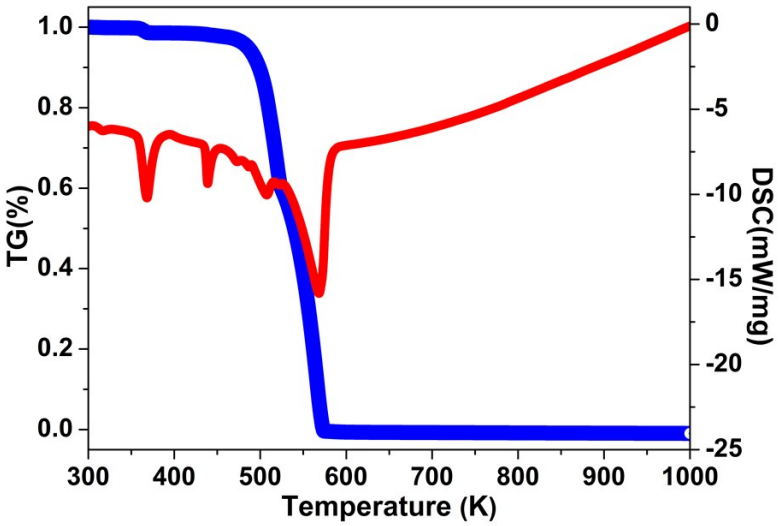

Figure S2. TG curve of **1**.

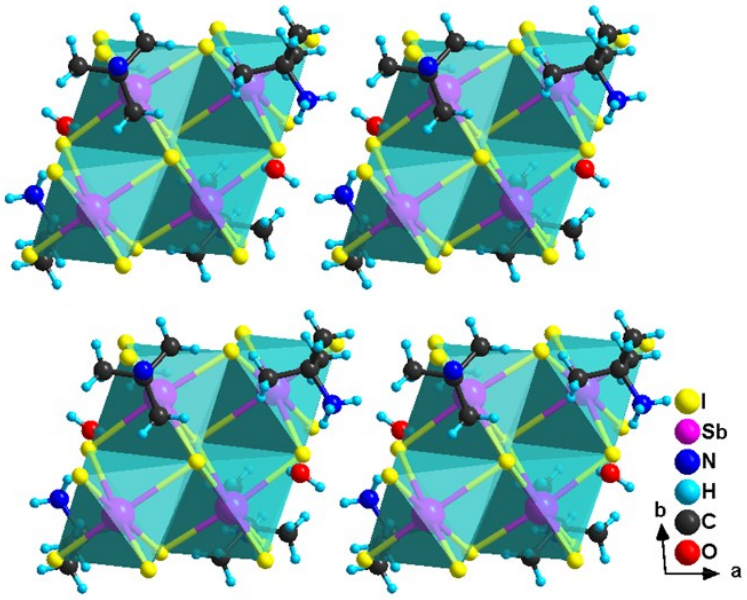

Figure S3. The packing structure of **1** viewed along the c-axis direction.

Table S1. Crystal structure and refinement detail of **1.**

Empirical formula	$[(CH_3)_3CNH_2]_4[Sb_4I_{16}].\ 2H_2O$
Formula weight	2814.05
Temperature/K	293.15
Crystal system	Triclinic
Space group	$P\ \bar{1}$
a/Å	11.142(5)
b/Å	11.794(4)
c/Å	13.105(4)
α/°,	65.193(13),
β/°,	77.627(17)
γ/°	89.043(16)
Volume/Å^3	1521.6(9)
Z/ρ_{calc} (mg/mm^3)	1 /3.110
m/mm^{-1}	9.892
F(000)	1224.0
Theta range for data collection	5.13 to 55.05°
Index ranges	-14 ≤ h ≤ 14,-15 ≤ k ≤ 15, -17 ≤ l ≤ 17
Reflections collected	47233
Independent reflections	6814 [R_{int} = 0.0563]
Data/restraints/parameters	6814/0/200
Goodness-of-fit on F^2	1.140
Final *R* indexes [$I>2\sigma(I)$]	R_1 = 0.0270, wR_2 = 0.0584
Final R indexes [all data]	R_1 = 0.0350, wR_2 = 0.0646

Table S2. Bond lengths for **1.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I_1	Sb_1	2.8031(8)	I_7	Sb_2	2.8761(9)
I_2	Sb_1	2.8061(9)	I_8	Sb_2	2.8995(8)
I_3	Sb_1	3.1329(12)	N_3	C_{0AA}	1.521(6)
I_3	Sb_2	3.2281(10)	C_{0AA}	C_1	1.513(8)
I_4	Sb_1	3.3810(10)	C_{0AA}	C_2	1.500(9)
I_4	Sb_1	3.3560(9)	C_{0AA}	C_4	1.521(8)
I_4	Sb_2	3.3378(13)	N_2	C_5	1.514(7)
I_5	Sb_1	2.9530(12)	C_5	C_6	1.541(10)
I_5	Sb_2	3.2066(9)	C_5	C_7	1.510(9)
I_6	Sb_2	2.8109(11)	C_5	C_8	1.502(10)

Table S3. Bond angles for **1**

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Sb1	I3	Sb2	96.79(3)	I6	Sb2	I7	94.57(3)
Sb1[1]	I4	Sb1	88.86(3)	I6	Sb2	I8	94.89(3)
Sb2	I4	Sb1	87.07(2)	I7	Sb2	I3	176.012(14)
Sb2	I4	Sb1	90.13(3)	I7	Sb2	I4	89.97(3)
Sb1[1]	I5	Sb2	96.85(3)	I7	Sb2	I5	93.45(3)
I1	Sb1	I2	90.21(3)	I7	Sb2	I8	89.97(3)
I1	Sb1	I3	92.02(3)	I8	Sb2	I3	89.32(3)
I1	Sb1	I4	89.96(3)	I8	Sb2	I4	92.55(3)
I1	Sb1	I5	91.94(3)	I8	Sb2	I5	176.324(14)
I2	Sb1	I3	90.01(3)	C1	C0AA	N3	106.5(5)
I2	Sb1	I4	176.934(14)	C1	C0AA	C4	111.5(5)
I2	Sb1	I5	93.35(3)	C2	C0AA	N3	106.7(5)
I3	Sb1	I4	86.92(3)	C2	C0AA	C1	114.1(6)
I5[1]	Sb1	I3	174.793(14)	C2	C0AA	C4	110.9(6)
I5[1]	Sb1	I4	89.70(3)	C4	C0AA	N3	106.7(4)
I3	Sb2	I4	86.14(3)	N2	C5	C6	105.4(6)
I5	Sb2	I3	87.18(3)	C7	C5	N2	107.3(5)
I5	Sb2	I4	86.11(2)	C7	C5	C6	110.7(6)
I6	Sb2	I3	89.40(3)	C8	C5	N2	106.7(5)
I6	Sb2	I4	171.272(16)	C8	C5	C6	112.3(6)
I6	Sb2	I5	86.18(3)	C8	C5	C7	113.7(7)