Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Surfactant-Thermal Method to Prepare Crystalline Thioantimonate for High-Performance Lithium-ion Batteries

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Supporting Information

Table S1. Crystallographic data and structure refinement for **1**

	1
Chemical formula	$C_2NH_7Sb_4S_8$
Formula mass	788.57
CCDC number	1430117
Crystal system	Orthorhombic
Space group	*Ama*2
a (Å)	10.0371(4)
b (Å)	26.6752(13)
c (Å)	5.9349(3)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
V (Å^3)	1589.02(13)
Z	4
D_{cal} (g/cm^3)	3.296
Theta (deg)	2.54-25.00
GOF on F^2	1.096
R_1, $wR_2[I > 2\sigma(I)]$	0.0505, 0.1554
R_1, wR_2 (all data)	0.0519, 0.1570

$^a R_1 = \sum \left| |F_o| - |F_c| \right| / \sum |F_o|$. $^b wR_2 = \left[\sum w \left(F_o^2 - F_c^2 \right)^2 / \sum w \left(F_o^2 \right)^2 \right]^{1/2}$.

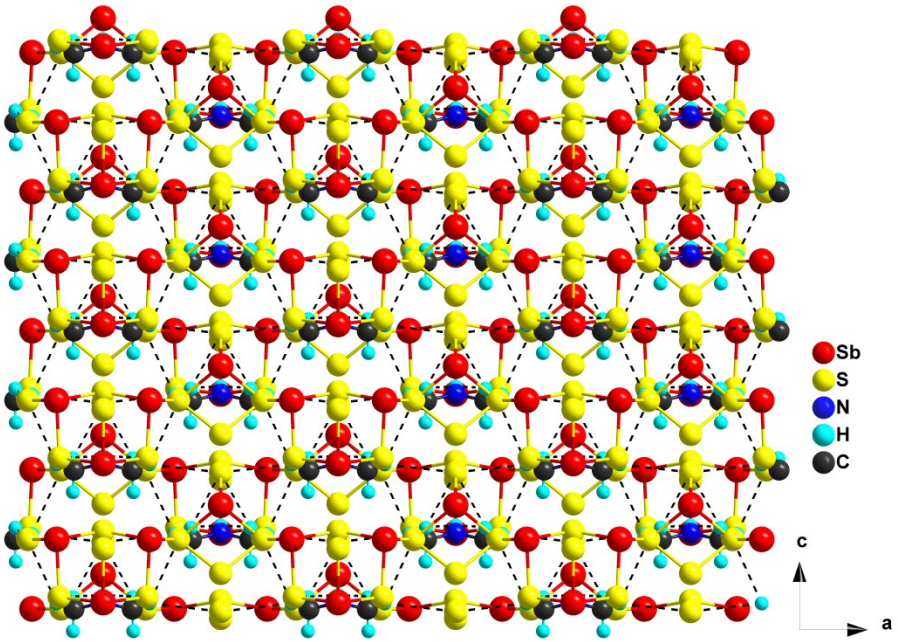

Fig. S1. The pseudo-2D network of compound **1** viewed along the *b* direction. H-bonding interactions are shown in dotted lines.

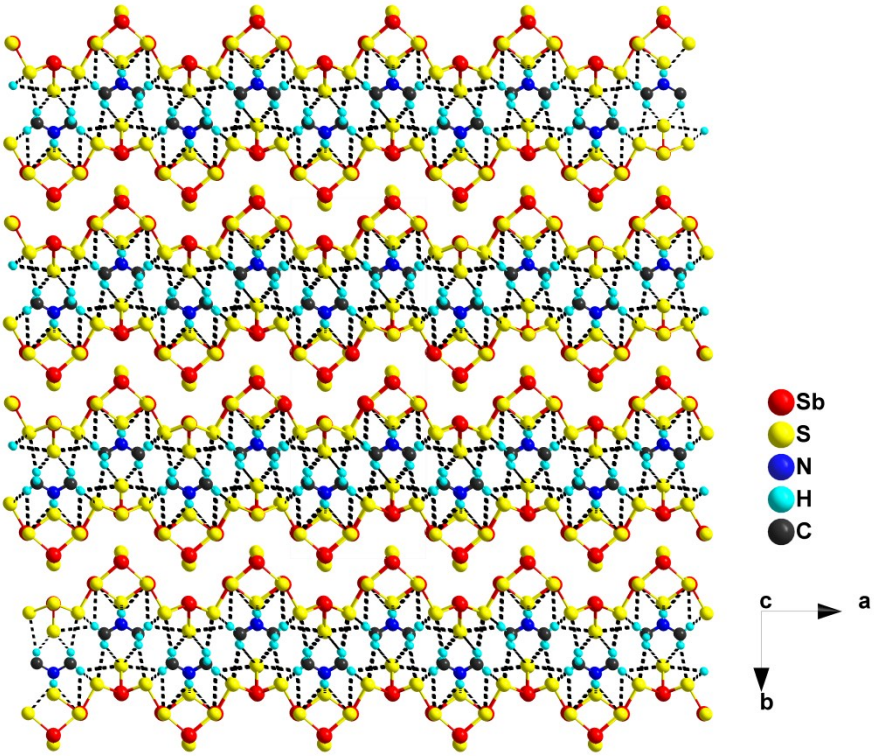

Fig. S2. Packing diagram of **1** viewed along the *c* direction. H-bonding interactions are shown in dotted lines.

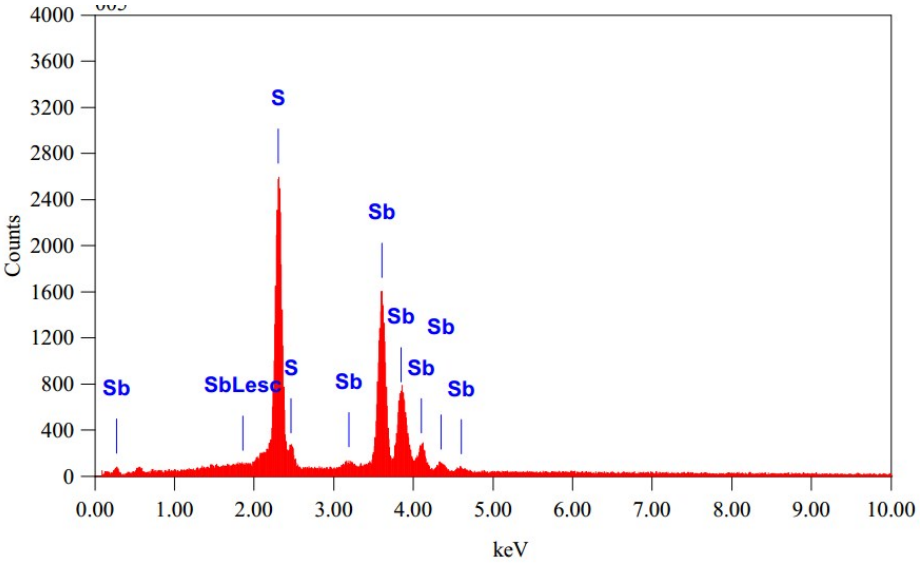

Fig. S3. The energy dispersive X-ray (EDX) spectroscopy of **1**

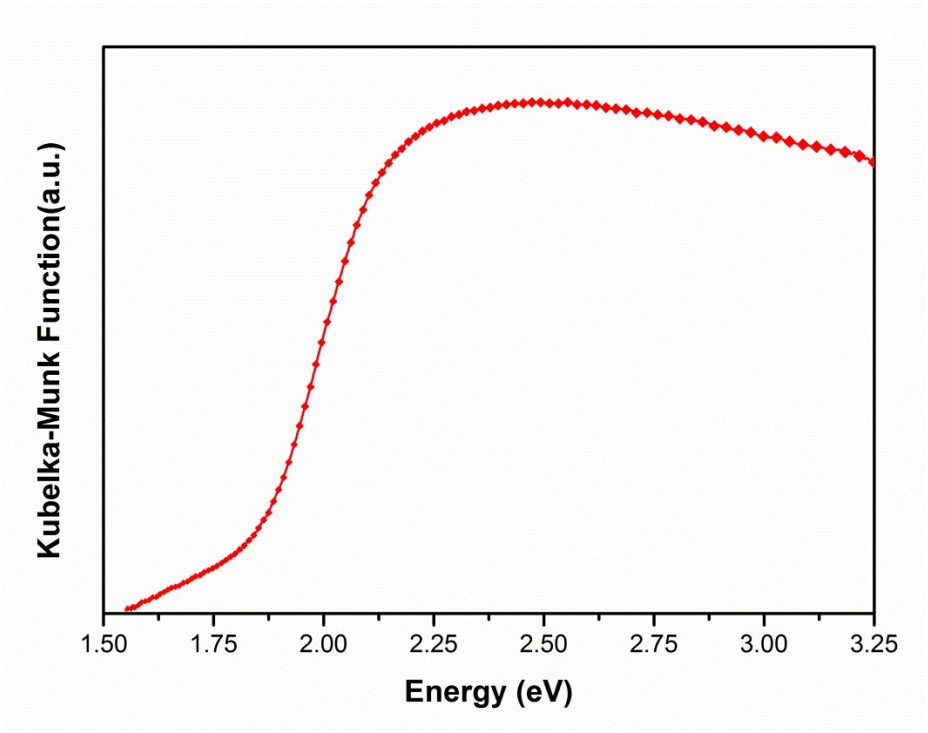

Fig. S4. Solid-state optical absorption spectrum of **1**

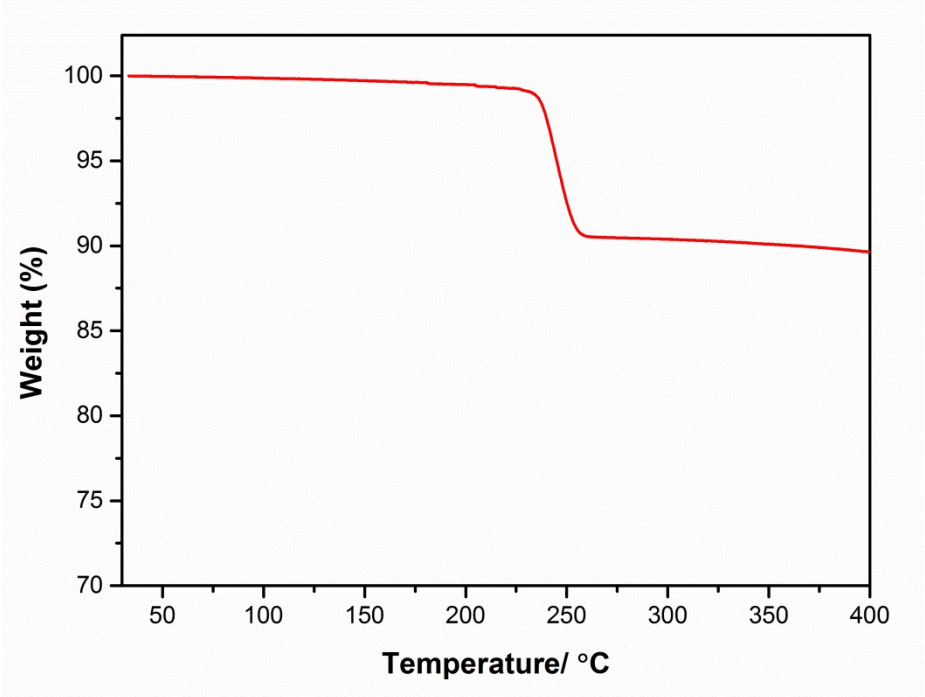

Fig. S6. TGA curve for compound **1**.