Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

$(C_6H_{15}N_3)_{1.3}(NH_4)_{1.5}H_{1.5}In_3SnS_8$: A layered metal sulfide based on supertetrahedral T2 clusters with photoelectric response and ion exchange property

Lu Yang,[a,b] Xin Wen,[a,b] Tian Yang,[a,b] Qian-Qian Hu,[b,c] Jia-Ting Liu,[a,b] Hai-Yan Yin,[a,b] Abdusalam Ablez,[a,b] Mei-Ling Feng,[b,c,*] and Xiao-Ying Huang[b,c,*]

[a] College of Chemistry, Fuzhou University, Fuzhou 350116, Fujian, China

Email: fml@fjirsm.ac.cn; xyhuang@fjirsm.ac.cn

[b] State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China.

[c] University of Chinese Academy of Sciences, Beijing, 100049, China

Table S1 Selected bond lengths (Å) and bond angles (°) for **1** at 293 K.

In(1)-S(1)	2.442(2)
In(1)-S(3)	2.4470(19)
In(1)-S(4)	2.444(3)
In(1)-S(5)	2.450(3)
In(2)-S(5)#2	2.442(3)
In(2)-S(4)#1	2.443(3)
In(2)-S(1)	2.451(2)
In(2)-S(2)	2.444(2)
S(1)-In(1)-S(3)	111.69(7)
S(1)-In(1)-S(4)	111.85(11)
S(5)-In(1)-S(5)	108.05(10)
S(3)-In(1)-S(5)	107.53(10)
S(4)-In(1)-S(3)	111.43(9)
S(4)-In(1)-S(5)	105.96(9)
S(2)-In(2)-S(1)	111.28(7)
S(4)#1-In(2)-S(1)	111.60(10)
S(4)#1-In(2)-S(1)	111.93(9)
S(5)#2-In(2)-S(1)	107.84(10)
S(5)#2-In(2)-S(2)	108.41(10)
S(5)#2-In(2)-S(4)#1	105.48(9)
In(1)-S(1)-In(2)	104.94(8)
In(2)#1-S(2)-In(2)	105.09(12)
In(1)#1-S(3)-In(1)	104.96(12)
In(2)#1-S(4)-In(1)	104.90(11)
In(2)#3-S(5)-In(1)	106.53(10)

Symmetry codes: #1 1-*x*,+*y*,1/2-*z*; #2 3/2-*x*,1/2+*y*,1/2-*z*; #3 3/2-*x*,-1/2+*y*,1/2-*z*

Table S2 Atomic coordinates (× 10^4), equivalent isotropic displacement parameters (Å^2 × 10^3), SOFs, and atomic sites for **1**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	*U*(eq)	SOF	Site
In(1)	0.64107(5)	0.05761(5)	0.31591(3)	0.0370(2)	0.75	8f
In(2)	0.60757(5)	0.30606(5)	0.18435(3)	0.0387(2)	0.75	8f
Sn(1)	0.64107(5)	0.05761(5)	0.31591(3)	0.0370(2)	0.25	8f
Sn(2)	0.60757(5)	0.30606(5)	0.18435(3)	0.0387(2)	0.25	8f
S(1)	0.75966(19)	0.1820(2)	0.25070(13)	0.0473(6)	1	8f
S(2)	0.500000	0.4409(3)	0.250000	0.0507(9)	1	4e
S(3)	0.500000	-0.0776(3)	0.250000	0.0463(8)	1	4e
S(4)	0.5340(3)	0.1811(3)	0.38704(13)	0.0670(8)	1	8f
S(5)	0.7842(3)	-0.0697(3)	0.38579(13)	0.0660(8)	1	8f

Table S3 EDS analysis results for **1**.

	S	Sn	In
Atomic %	64.27 ± 0.27	8.08 ± 1.18	27.65 ± 1.24

Table S4 Ion exchange experimental results of Sr^{2+} ions capture by **1** (*V*/*m* = 1000 mL/g; at 60 °C; 12 h contact time).

C_0^{Sr} (mg/L)	C_e^{Sr} (mg/L)	q^{Sr} (mg/g)	R^{Sr} (%)
44.00	0.56	43.44	98.73
103.24	0.29	102.94	99.72

Where C_0 and q_e (mg·g^{-1}) are concentrations of the target ions (mg/L) at the initial state and equilibrium state, respectively; *R* (%) and q_e (mg·g^{-1}) are removal rate and equilibrium adsorption amount q_e (mg·g^{-1}), respectively.

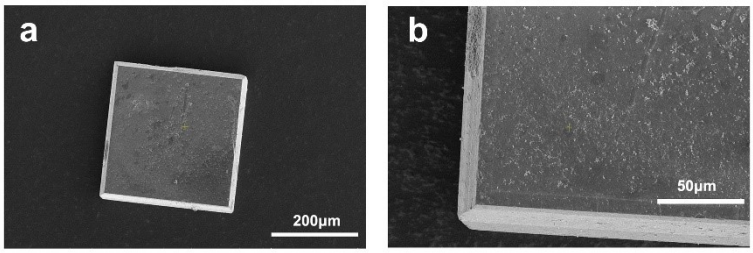

Fig. S1 The SEM images for the crystal of **1**. (a) The whole crystal; (b) the partial crystal.

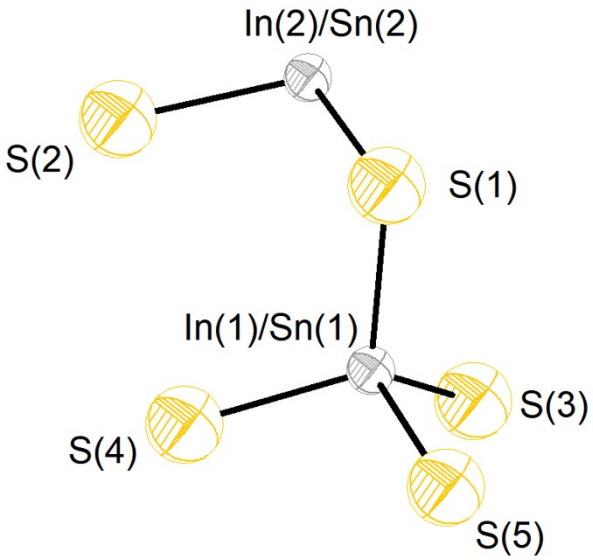

Fig. S2 *ORTEP* plot (50% ellipsoid probability) of the anionic part of the crystallographically asymmetric unit of **1**.

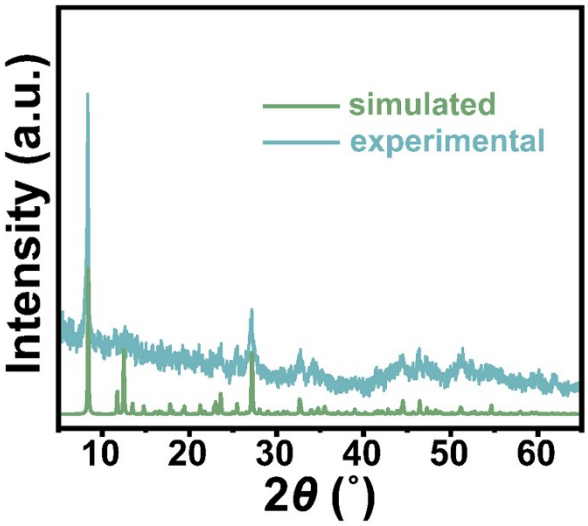

Fig. S3 Experimental and simulated powder XRD patterns for **1**.

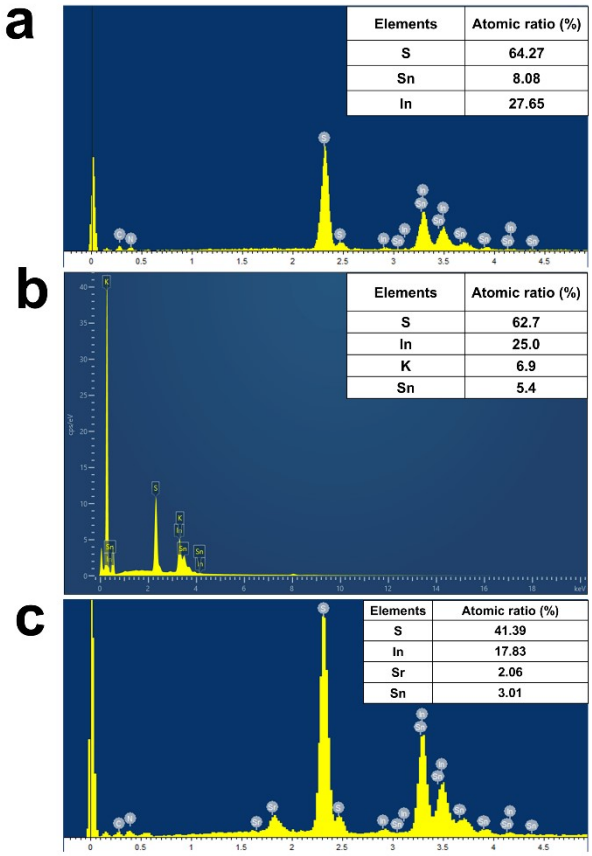

Fig. S4 The EDS of **1** (a), **1-K** (b), and **1-Sr** (c).

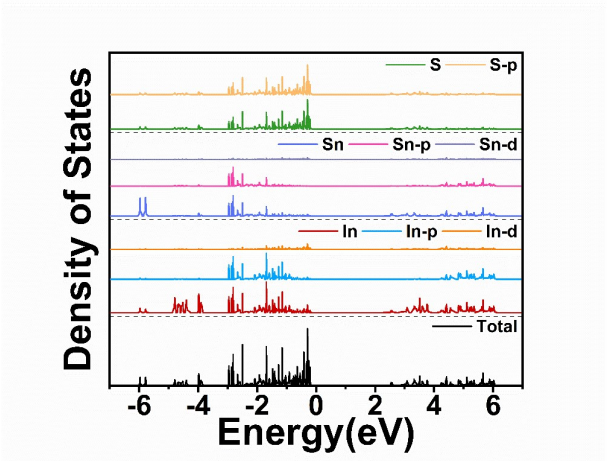

Fig. S5 The calculated orbital-resolved DOSs of **1**.