Supporting Information for

Solvothermal synthesis and characterization of thioindate-thioantimonates with transition-metal complexes: the first examples of the incorporation of transition metal ions into In-S-Sb framework

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Table S1 Some important bond lengths (Å) and angles (°) for **1-3**.

		1	
Sb1-S	2.454(5)-2.460(5)	Sb2-S	2.417(5)-2.447(5)
In1-S	2.445(5)-2.492(5)	In2-S	2.422(4)-2.491(5)
Ni1-N	2.03(15)-2.17(5)	S-Sb1-S	94.76(18)-96.66(18)
S3-Sb2-S	91.31(18)-100.8(2)	S-In1-S	105.20(19)-113.78(18)
S-In2-S	103.14(18)-117.29(17)	N-Ni1-N	77.4(10)-172.6(9)
		2	
Sb1-S	2.4212(17)−2.4288(18)	Sb2-S	2.4263(19)−2.4638(19)
Sb3-S	2.4311(19)−2.447(2)	In1-S	2.4212(19)−2.4942(19)
In2-S	2.4379(19)−2.470(2)	In3-S	2.4328(17)−2.4721(19)
Ni1-N	2.188(7)−2.217(6)	Ni2-N	2.155(14)−2.29(2)
S-Sb1-S	92.75(6)−98.89(7)	S-Sb2-S	91.26(7)−95.92(7)
S-Sb3-S	90.87(7)−101.22(8)	S-In1-S	101.85(6)−123.84(7)
S-In2-S	103.41(7)−114.16(7)	S-In3-S	107.09(7)−112.56(6)
N-Ni1-N	77.5(3)−168.4(3)	N-Ni2-N	79.1(9)−173.4(6)
		3	
Sb1-S	2.413(6)−2.435(6)	In1-S	2.463(6)−2.484(7)
Co1-N	2.07(2)− 2.21(2)	Co1-S	2.318(6)
S-Sb1-S	90.6(2)− 99.5(2)	S-In1-S	97.68(18)−119.5(2)
N-Co1-N	78.0(8)−130.0(9)	N-Co1-S	95.5(5)−173.7(5)

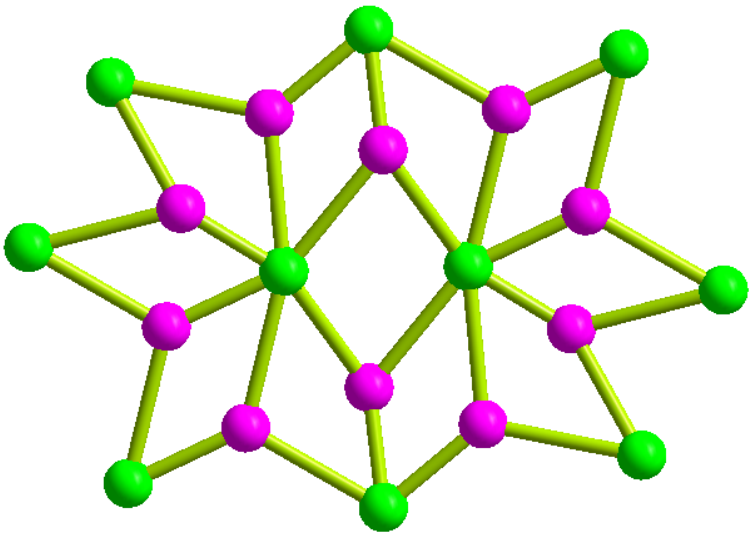


Figure S1 Topology of the $[In_2Sb_2S_7]^{2n-}_n$ layer in **1**(green/pink: $[In_2S_7]$/[$[SbS_3]$ nodes).

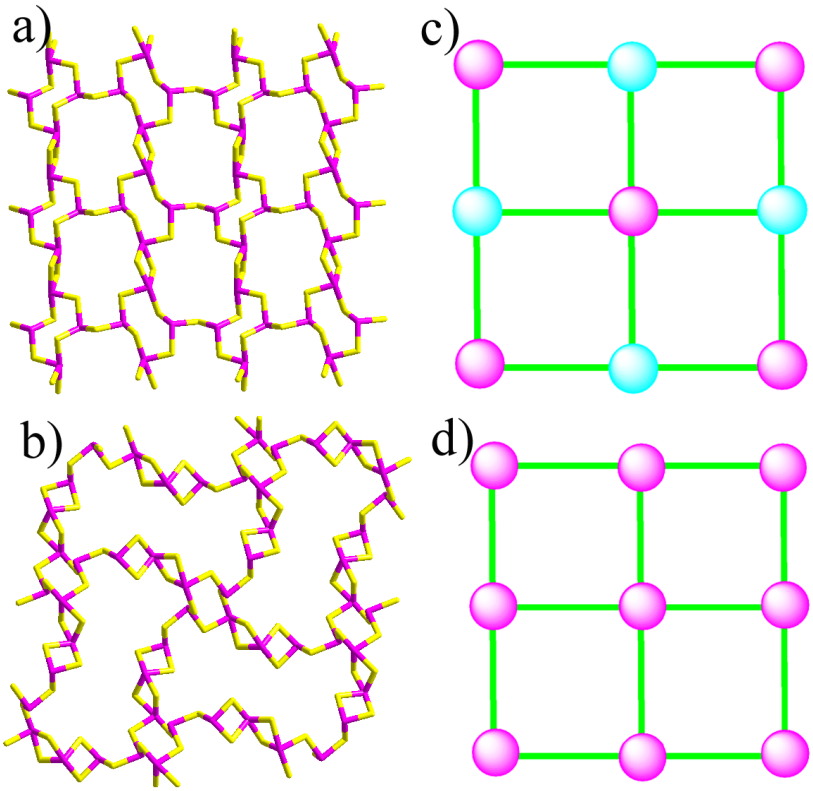


Figure S2 View of 2-D $[Sb_4S_7]^{2n-}_n$ layers (a,b). Topology of the $[Sb_4S_7]^{2n-}_n$ layers (c, blue/pink:$[Sb_2S_5]$/$[Sb_2S_6]$ nodes; d, pink:$[Sb_4S_9]$ nodes).

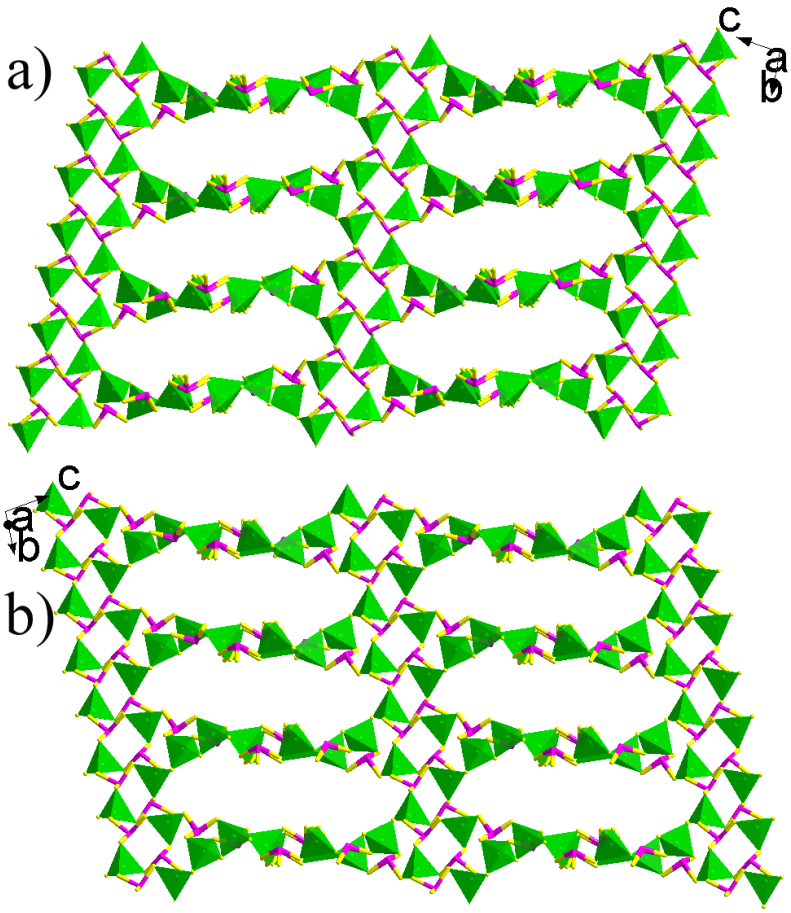
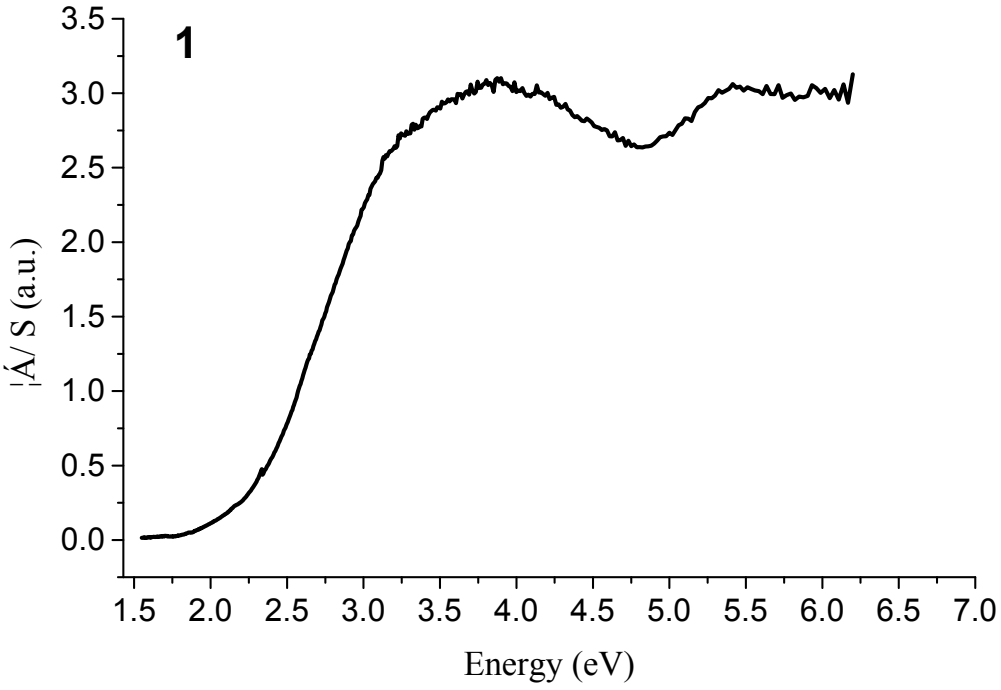
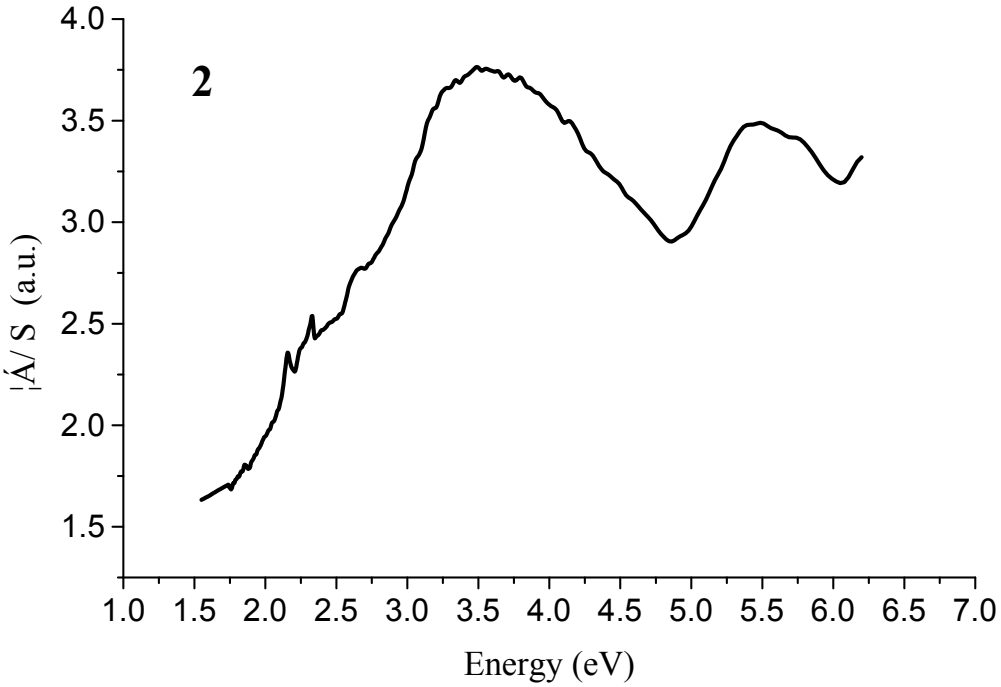


Figure S3 View of 3-D In–S–Sb open-framework in **2** along [ī10] and [1ī0].





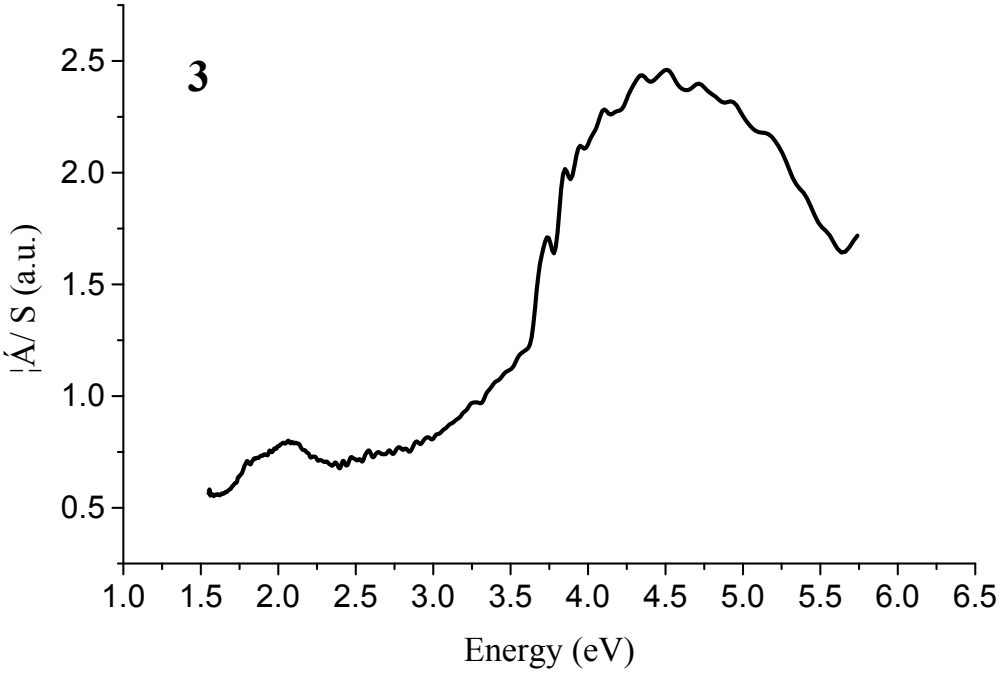


Figure S4 The solid-state UV/Vis absorption spectra of **1**-**3**.

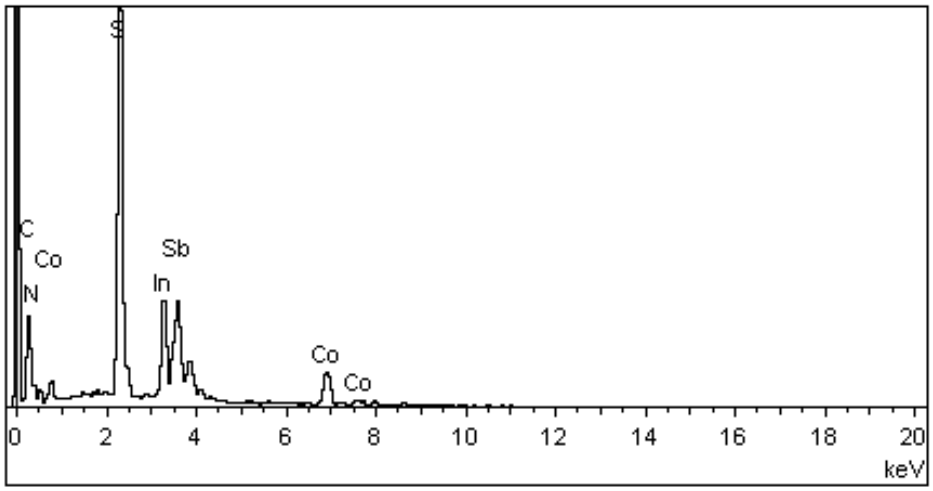


Figure S5 EDS spectrum of **3**.

The energy dispersive spectroscopy (EDS) analyses show that molar ratios of In:Sb:Co:S are 1.05:1.03:1.07:4.05 for **3**, consistent with the stoichiometry.

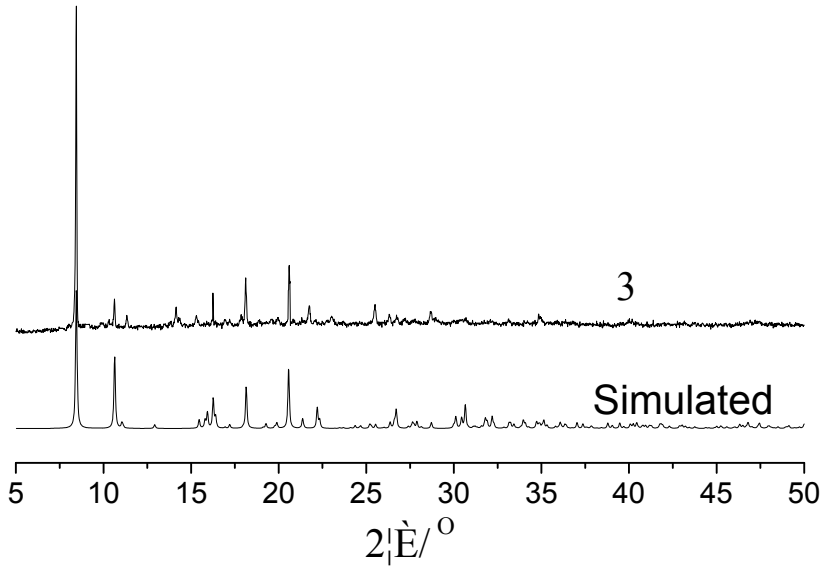


Figure S6 Simulated and experimental powder XRD patterns of **3** (The simulated XRD pattern is slightly different from the measured one. It means that **3** is sensible to the moisture and air).