Electronic Supplementary Material (ESI) for Dalton Transactions

Solvothermal synthesis and characterization of two 2-D layered germanium thioantimonates with transition-metal complexes

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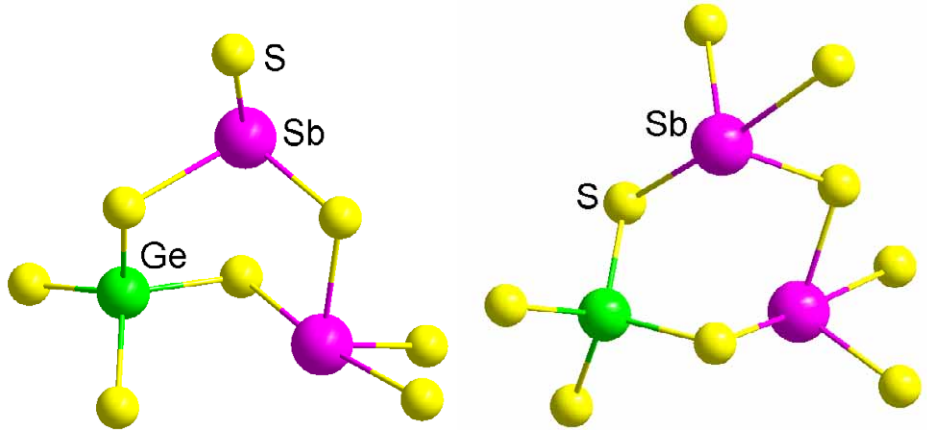
Table S1. Selected Bond Lengths (Å) and Angles (deg) for **1** and **2**.

		1	
Ge1-S1	2.147(6)	Sb1-S2	2.424(6)
Ge1-S3	2.173(6)	Sb1-S5	2.437(6)
Ge1-S4	2.254(6)	Sb1-S10#1	2.480(5)
Ge1-S2	2.279(6)	Sb2-S4	2.455(6)
Sb3-S7	2.374(6)	Sb2-S6	2.466(5)
Sb3-S8	2.397(7)	Sb2-S5	2.520(6)
Sb3-S6	2.484(5)	Sb4-S10	2.488(6)
Sb4-S9#2	2.377(5)	Sb4-S8	2.732(6)
Sb4-S9	2.777(5)	S2-Sb1-S5	100.1(2)
S1-Ge1-S3	119.9(2)	S2-Sb1-S10#1	94.9(2)
S1-Ge1-S4	111.4(2)	S5-Sb1-S10#1	89.30(19)
S3-Ge1-S4	104.5(2)	S4-Sb2-S6	92.48(18)
S1-Ge1-S2	108.2(2)	S4-Sb2-S5	98.0(2)
S3-Ge1-S2	105.0(2)	S6-Sb2-S5	89.73(18)
S4-Ge1-S2	107.0(2)	S7-Sb3-S8	102.3(2)
S10-Sb4-S9	88.89(18)	S7-Sb3-S6	96.22(19)
S8-Sb4-S9	172.37(19)	S8-Sb3-S6	98.1(2)
S10-Sb4-S8	94.58(19)	S9#2-Sb4-S10	100.1(2)
S9#2-Sb4-S9	84.01(17)	S9#2-Sb4-S8	88.70(19)
N9-Co2-N10	153.2(16)	N3-Co1-N4	95.8(7)
N7-Co2-N10	99.5(14)	N3-Co1-N6	92.6(7)
N9-Co2-N12	76.6(12)	N4-Co1-N6	102.7(7)
N7-Co2-N12	98.4(16)	N3-Co1-N1	99.5(7)
N10-Co2-N12	83.7(15)	N4-Co1-N1	156.2(7)
N9-Co2-N11	88.1(11)	N6-Co1-N1	94.7(7)
N7-Co2-N11	163.9(17)	N3-Co1-N2	81.0(7)
N10-Co2-N11	76.3(13)	N4-Co1-N2	85.4(7)
N12-Co2-N11	97(2)	N6-Co1-N2	170.2(7)
N9-Co2-N8	79.0(9)	N1-Co1-N2	79.2(7)
N7-Co2-N8	83.3(10)	N3-Co1-N5	168.0(7)
N10-Co2-N8	120.4(13)	N4-Co1-N5	78.2(7)
N12-Co2-N8	155.4(11)	N6-Co1-N5	78.8(7)
N11-Co2-N8	85.5(15)	N1-Co1-N5	89.6(7)
N9-Co2-N7	101.1(9)	N2-Co1-N5	108.6(7)
		2	
Sb1-S3	2.4315(12)	Ge1-S6	2.1365(13)
Sb1-S4	2.4585(12)	Ge1-S1	2.2153(13)

Sb1-S5#3	2.4658(12)	Ge1-S5	2.2511(12)
Sb2-S2	2.3873(13)	Ge1-S4	2.2633(12)
Sb2-S3	2.4682(13)	Sb2-S1	2.7659(11)
Sb2-S2#4	2.6959(12)	Mn1-N4	2.287(4)
Mn1-N5	2.265(4)	Mn1-N3	2.292(4)
Mn1-N6	2.277(5)	Mn1-N1	2.301(4)
Mn1-N2	2.280(5)	S6-Ge1-S1	116.17(5)
S3-Sb1-S4	100.29(5)	S6-Ge1-S5	110.22(5)
S3-Sb1-S5#3	90.04(5)	S1-Ge1-S5	108.97(6)
S4-Sb1-S5#3	91.22(5)	S6-Ge1-S4	117.09(6)
S2-Sb2-S3	102.77(5)	S1-Ge1-S4	101.70(4)
S2-Sb2-S2#4	88.23(4)	S5-Ge1-S4	101.37(5)
S3-Sb2-S2#4	85.12(4)	N5-Mn1-N6	77.00(16)
S2-Sb2-S1	83.82(4)	N5-Mn1-N2	100.98(16)
S3-Sb2-S1	91.50(4)	N6-Mn1-N2	101.7(2)
S2#4-Sb2-S1	170.47(4)	N5-Mn1-N4	93.57(14)
N2-Mn1-N3	92.15(15)	N6-Mn1-N4	94.33(19)
N4-Mn1-N3	76.95(13)	N2-Mn1-N4	160.38(17)
N5-Mn1-N1	97.99(16)	N5-Mn1-N3	161.87(17)
N6-Mn1-N1	174.27(17)	N6-Mn1-N3	88.21(16)
N2-Mn1-N1	76.36(17)	N3-Mn1-N1	97.22(16)
N4-Mn1-N1	88.72(17)		

Symmetry transformations used to generate equivalent atoms: (#1) $-x+1/2$, $y-1/2$, z; (#2) $-x+1$, $-y+3$, $-z+1$; (#3) $x-1/2$, y, $-z-1/2$; (#4) $-x$, $-y-1$, $-z$.



a b

Figure S1 The structures of $[GeSb_2S_8]$ (a) and $[GeSb_2S_9]$ cluster (b).

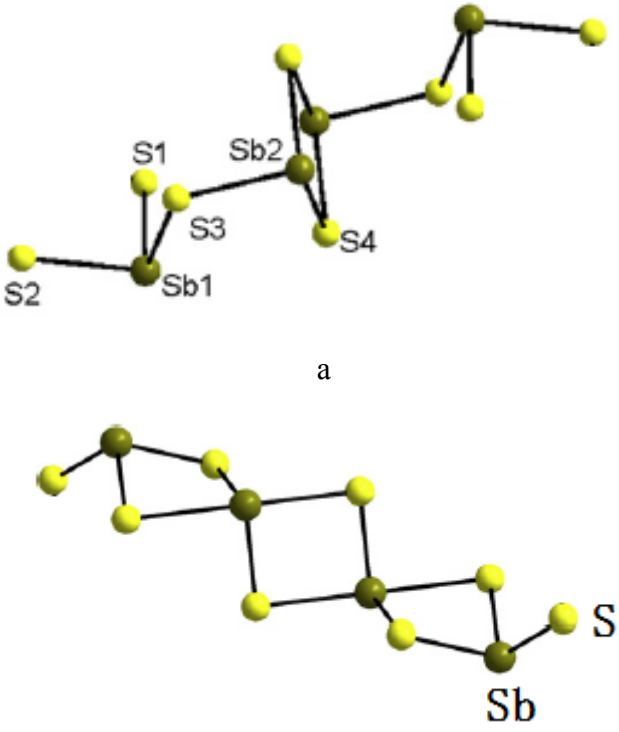


Figure S2 The structures of $[Sb_4S_8]^{4-}$ anion (a) in $\{[In(C_6H_{14}N_2)_2]_2Sb_4S_8\}Cl_2$ and $[Sb_4S_8]^{4-}$ anion in $[M(tren)]_2[Sb_4S_8]$ (M = Zn, Co) (b).

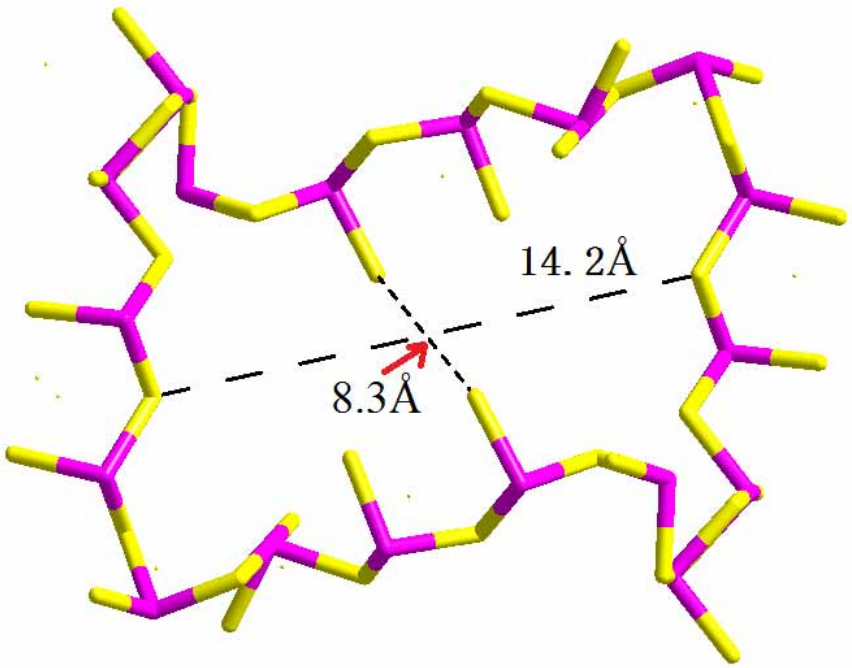


Figure S3 The rectangular 18-MR ring.

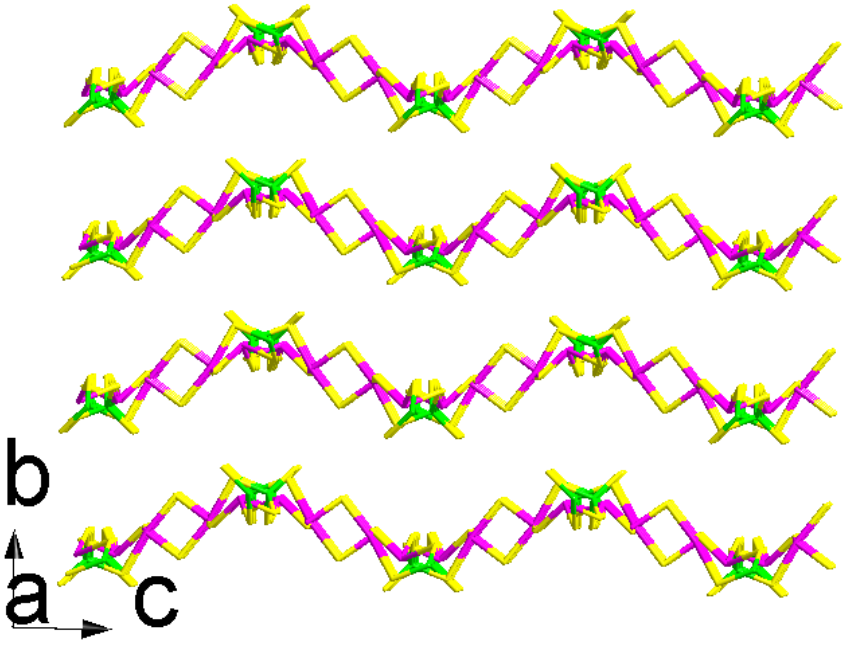


Figure S4 The adjacent layers stacked in a parallel fashion along the b-axis.

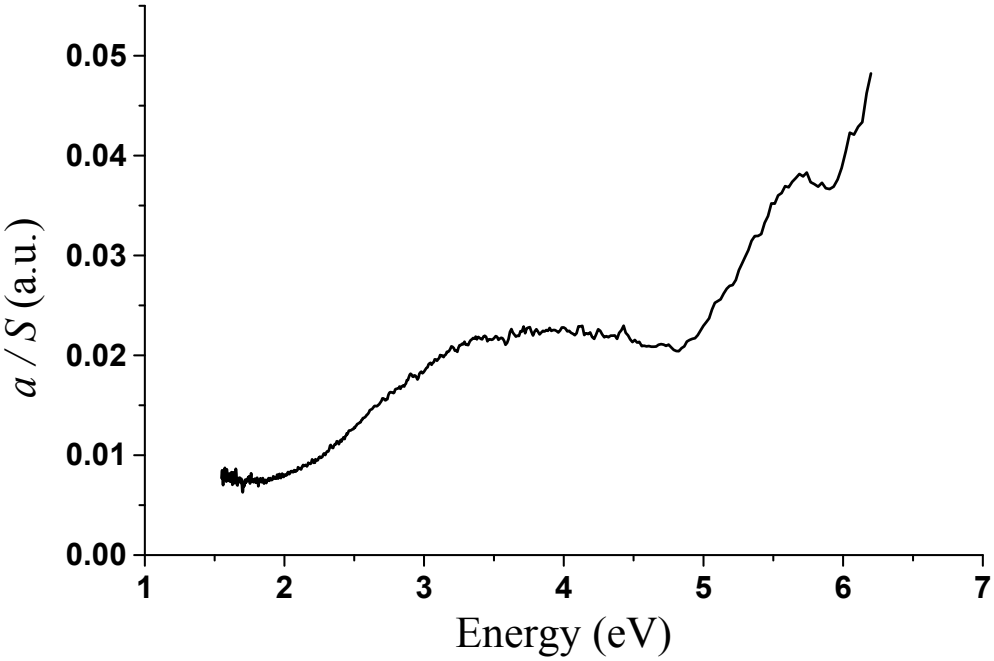


Figure S5 The diffuse reflection spectrum of **2**.

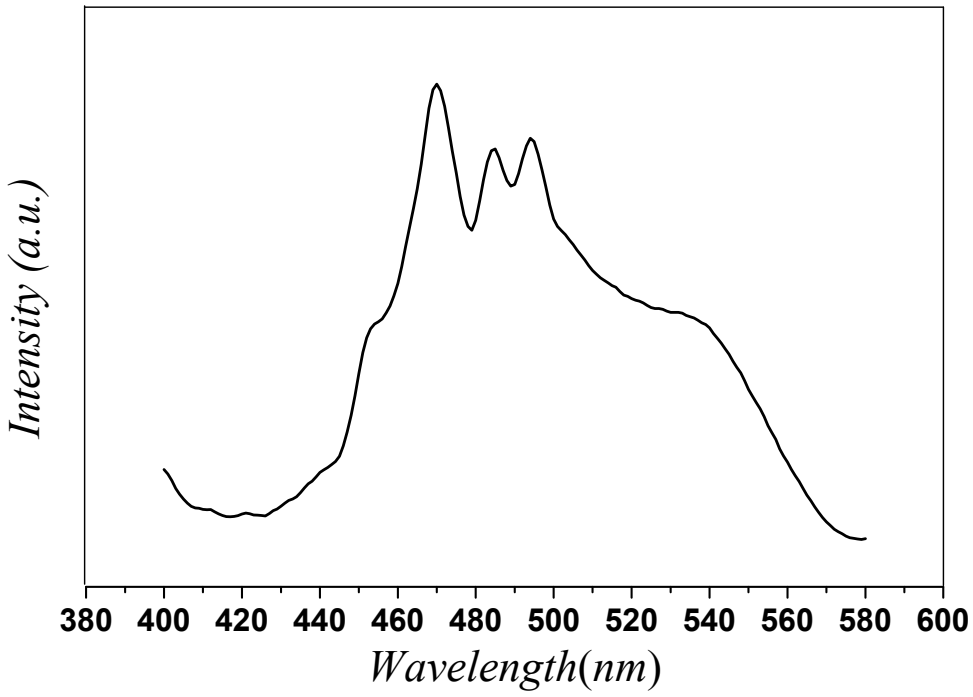
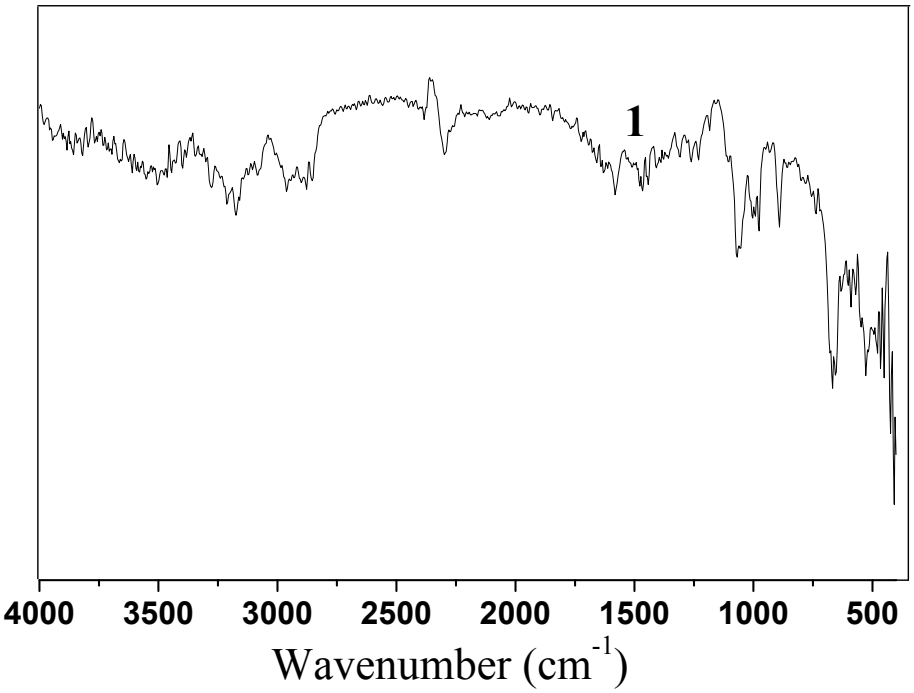


Figure S6 Solid-state photoluminescence of **2**.



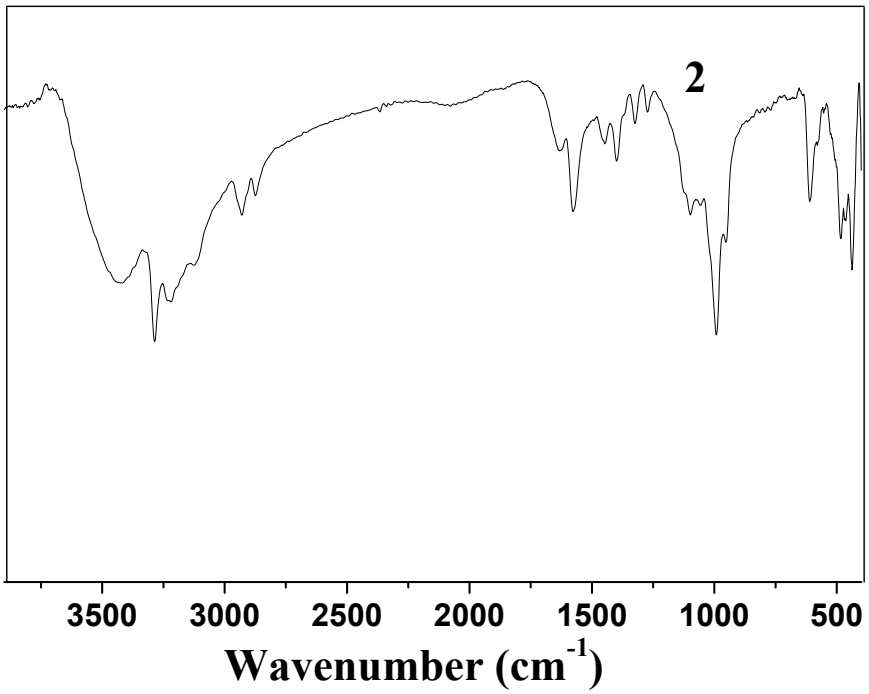


Figure S7 IR spectra of **1** and **2**.

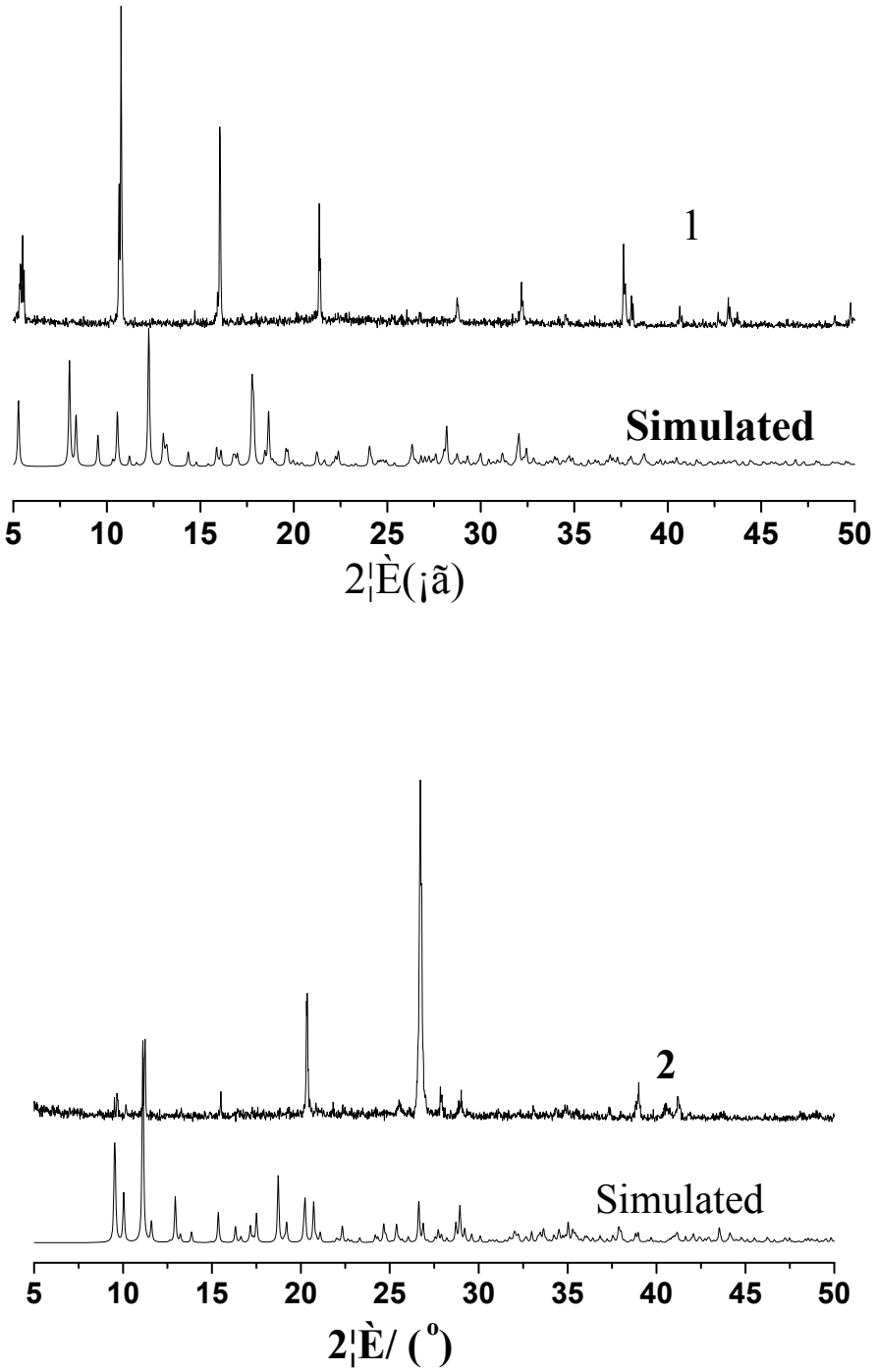


Figure S8 Experimental powder XRD pattern of **1** and **2**.

The experimental peak positions are in agreement with simulated XRD pattern, indicating the phase purity of **1** and **2**. The difference in reflection intensity between experimental and simulated XRD patterns is probably due to the preferred orientation effect of the powder sample during collection of the experimental XRD data.