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Supporting information for

Noncentrosymmetric sulfides $A_2Ba_6MnSn_4S_{16}$ (A = Li, Ag): Syntheses, structures, and properties

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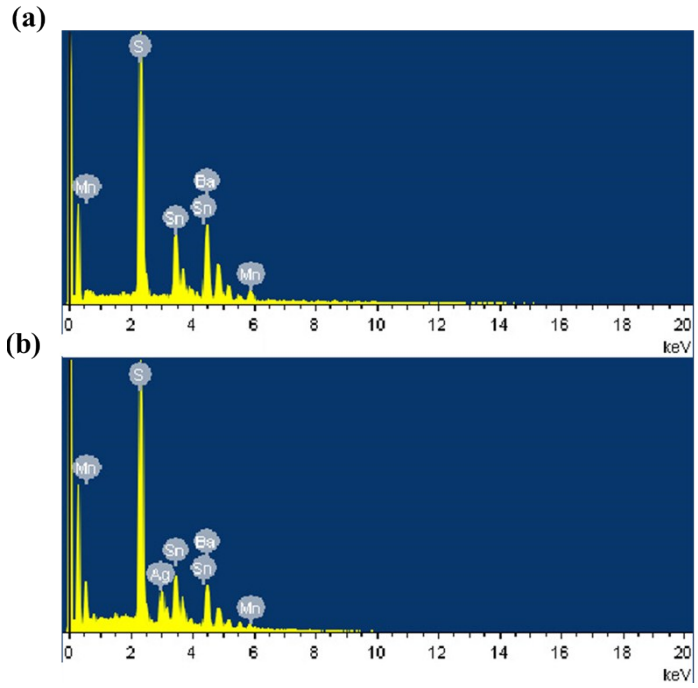

Figure S1. EDS spectrum for compound **1** (a) and **2** (b).

Table S1. Atomic coordinates, equivalent isotropic displacement parameters and occupancies of compound **1** and **2**.

Atom	Oxidation	Wyckoff	x	y	z	U(eq)	sof
				1			
Ba1	+2	24*d*	0.5000	0.2500	0.9850(1)	0.01744(9)	1
Sn1	+4	16*c*	0.4775(1)	0.5225(1)	1.0225(1)	0.01062(2)	1
Mn1	+2	12*a*	0.3750	0.0000	1.2500	0.0150(7)	0.33
Li1	+1	12*a*	0.3750	0.0000	1.2500	0.0150(7)	0.67
S1	–2	16*c*	0.3655(1)	0.1345(1)	0.8655(1)	0.0180(3)	1
S2	–2	48*e*	0.4331(1)	0.0815(1)	1.1131(1)	0.0137(1)	1
				2			
Ba1	+2	24*d*	1.0000	0.7500	0.9828(1)	0.0182(1)	1
Sn1	+4	16*c*	1.0219(1)	1.0219(1)	1.0219(1)	0.0116(1)	1
Mn1	+2	12*b*	0.7500	0.6250	1.0000	0.008(3)	0.33

Ag1	+1	12*b*	0.7500	0.6250	1.0000	0.038(1)	0.67
S1	–2	16*c*	0.8641(1)	0.8641(1)	0.8641(1)	0.0172(4)	1
S2	–2	48*e*	0.8898(1)	0.5658(1)	0.9158(1)	0.0153(2)	1

Table S2. Selected bond lengths (Å) and angles (deg) for compound **1** and **2**.

1		**2**	
Ba1-S1×2	3.1233(5)	Ba1-S1×2	3.1391(7)
Ba1-S2×2	3.2420(8)	Ba1-S2×2	3.2234(10)
Ba1-S2×2	3.2907(8)	Ba1-S2×2	3.3071(10)
Ba1-S2×2	3.4551(8)	Ba1-S2×2	3.4948(10)
Sn1-S1	2.3539(14)	Sn1-S1	2.3505(17)
Sn1-S2×3	2.4002(8)	Sn1-S2×3	2.4044(9)
Li/Mn1-S2×4	2.4781(7)	Ag/Mn1-S2×4	2.5535(10)
S1-Sn1-S2×3	111.16(2)	S1-Sn1-S2×3	111.85(2)
S2-Sn1-S2×3	107.73(3)	S2-Sn1-S2×3	106.99(3)
S2-Li/Mn-S2×4	96.744(12)	S2-Li/Cd-S2×4	96.683(14)
S2-Li/Mn-S2×2	139.92(4)	S2-Li/Cd-S2×2	140.11(4)

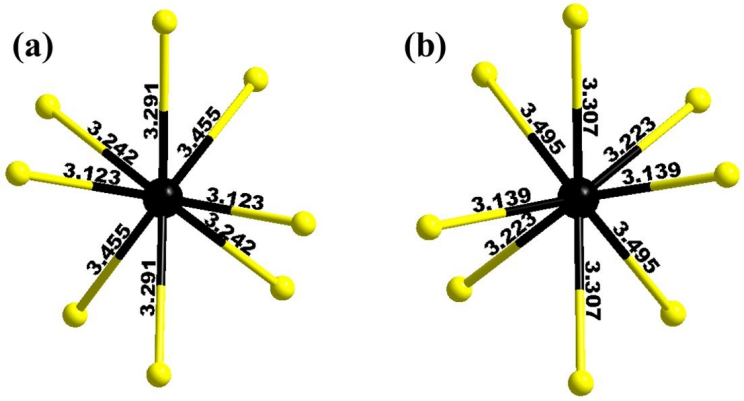

Figure S2. The environment of Ba atom in compound **1** (a) and **2** (b).

Table S3. Band Valence in compound **1** and **2**.

1		**2**	
atom	valence	atom	valence
Ba	2.13	Ba	2.08
Sn	4.12	Sn	4.10
Li	0.93	Ag	1.34
Mn	1.89	Mn	1.54

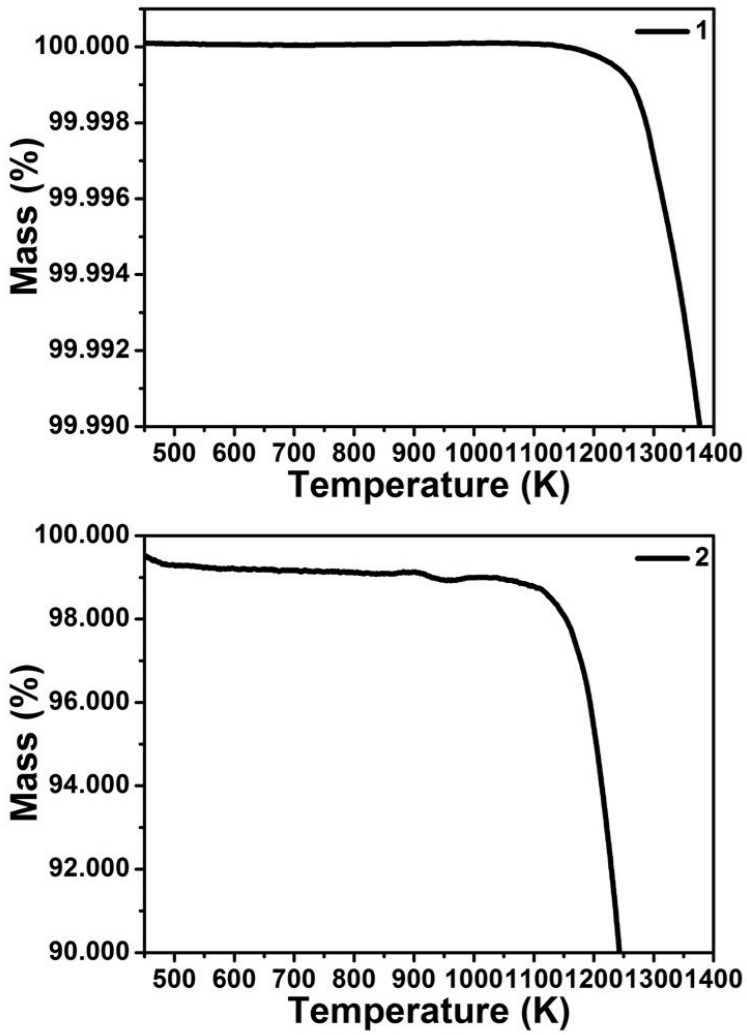

Figure S3. The TGA patterns of compound **1** (a) and **2** (b) under N_2 flow.

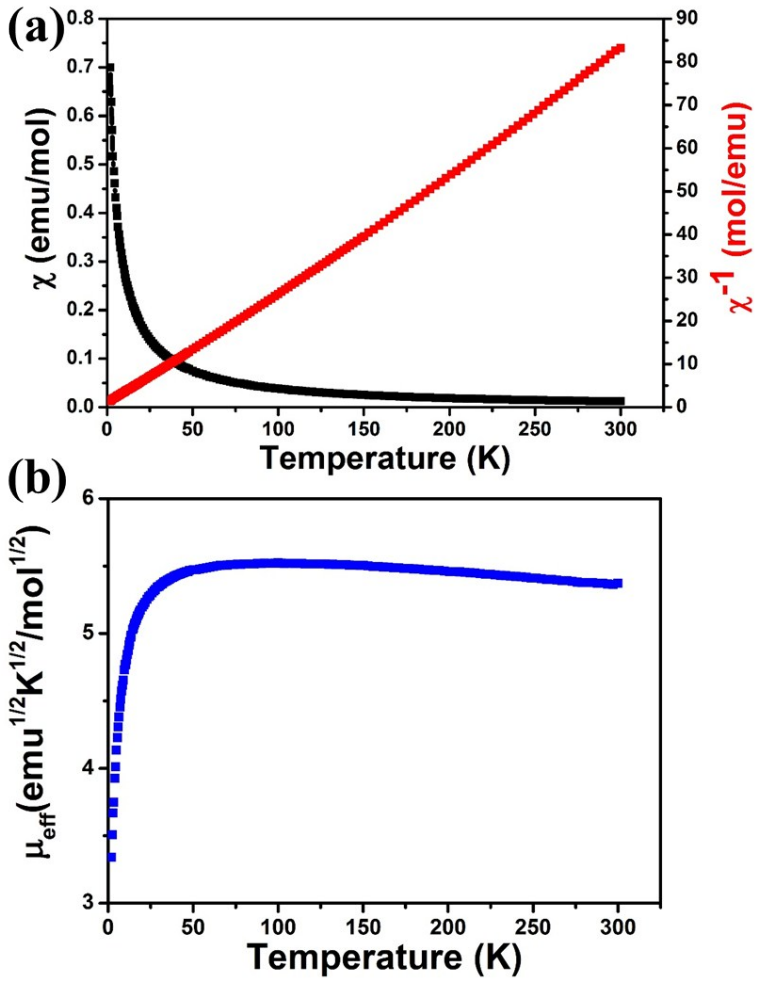

Figure S4. Temperature-dependence of the molar magnetic susceptibility (a, black), the inverse molar magnetic susceptibility (a, red) and the experimental effective magnetic moment (b) for compound **2**.