Syntheses, Crystal and Electronic Structures, and Physical Properties of Quaternary Semiconductors: $Ln_2Mn_3Sb_4S_{12}$ (Ln = Pr, Nd, Sm, Gd)

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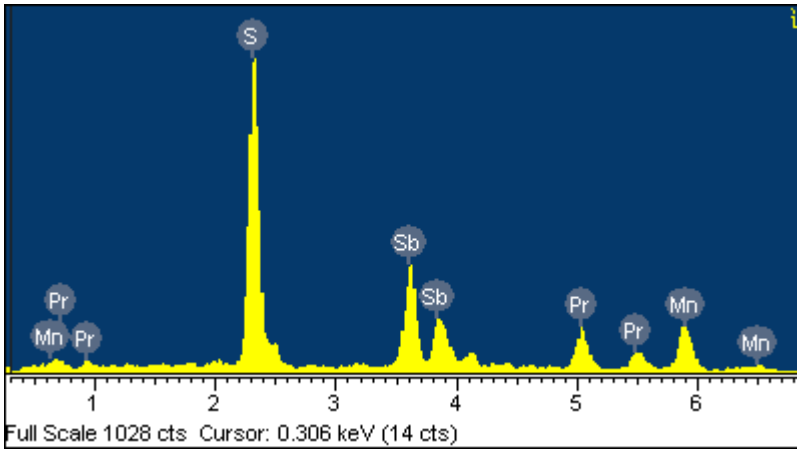

Figure S1. The EDX spectrum of $Pr_2Mn_3Sb_4S_{12}$.

Point-1

Element	Weight%	Atomic%	Formula
S K	32.14	61.38	12.94
Mn K	9.77	10.89	2.30
Sb L	36.25	18.24	3.84
Pr L	21.84	9.49	2
Totals	100.00		

Point-2

Element	Weight%	Atomic%	Formula
S K	31.18	60.31	11.72
Mn K	10.09	11.39	2.21
Sb L	35.35	18.01	3.50
Pr L	23.38	10.29	2
Totals	100.00		

Point-3

Element	Weight%	Atomic%	Formula
S K	26.79	54.56	11.12
Mn K	11.83	14.07	2.87
Sb L	40.19	21.56	4.40
Pr L	21.18	9.81	2
Totals	100.00		

Point-4

Element	Weight%	Atomic%	Formula
S K	31.68	60.89	13.09
Mn K	9.71	10.90	2.34
Sb L	37.35	18.91	4.07
Pr L	21.26	9.30	2
Totals	100.00		

Point-5

Element	Weight%	Atomic%	Formula
S K	31.10	60.03	12.47
Mn K	10.45	11.77	2.44
Sb L	36.52	18.56	3.85
Pr L	21.93	9.63	2
Totals	100.00		

Average formula: $Pr_2Mn_{2.4(3)}Sb_{3.9(3)}S_{12.3(8)}$

Table S1. Atomic coordinates and equivalent isotropic displacement parameters of $Nd_2Mn_3Sb_4S_{12}$.

atom	symmetry	*x*	*y*	*z*	*U*(eq)
Nd	*4i*	0.24010(5)	0	0.13447(7)	0.0157(3)
Sb1	*4i*	0.10605(7)	0	0.55078(9)	0.0256(3)
Sb2	*4i*	0.46367(8)	0	0.1877(1)	0.0279(3)
Mn1	*4i*	0.1990(1)	0	0.3789(2)	0.0140(5)
Mn2	*2a*	0	0	0	0.0238(8)
S1	*4i*	0.0575(2)	0	0.1967(3)	0.0130(8)
S2	*4i*	0.6028(2)	0	0.0234(3)	0.0110(7)
S3	*4i*	0.8306(2)	0	0.1057(3)	0.0111(7)
S4	*4i*	0.4111(2)	0	0.3480(3)	0.0127(8)
S5	*4i*	0.2554(2)	0	0.7073(3)	0.0114(7)
S6	*4i*	0.3475(2)	0	0.5505(3)	0.0158(8)

Table S2. Atomic coordinates and equivalent isotropic displacement parameters of $Sm_2Mn_3Sb_4S_{12}$.

atom	symmetry	*x*	*y*	*z*	*U*(eq)
Sm	*4i*	0.23997(7)	0	0.13328(9)	0.0154(3)
Sb1	*4i*	0.10565(9)	0	0.5510(1)	0.0248(4)
Sb2	*4i*	0.4628(1)	0	0.1894(1)	0.0260(4)
Mn1	*4i*	0.1987(2)	0	0.3779(2)	0.0143(7)
Mn2	*2a*	0	0	0	0.025(1)
S1	*4i*	0.0561(3)	0	0.1966(4)	0.014(1)
S2	*4i*	0.6041(3)	0	0.0246(4)	0.0118(9)
S3	*4i*	0.8298(3)	0	0.1054(4)	0.013(1)
S4	*4i*	0.4107(3)	0	0.3460(4)	0.014(1)
S5	*4i*	0.2549(3)	0	0.7081(4)	0.014(1)
S6	*4i*	0.3480(3)	0	0.5503(4)	0.017(1)

Table S3. Atomic coordinates and equivalent isotropic displacement parameters of $Gd_2Mn_3Sb_4S_{12}$.

atom	symmetry	*x*	*y*	*z*	*U*(eq)
Gd	*4i*	0.24146(6)	0	0.13503(7)	0.0189(3)
Sb1	*4i*	0.10642(7)	0	0.5515(1)	0.0216(4)
Sb2	*4i*	0.46171(9)	0	0.1846(1)	0.0252(4)
Mn1	*4i*	0.1990(2)	0	0.3787(2)	0.0143(6)
Mn2	*2a*	0	0	0	0.027(1)
S1	*4i*	0.0560(3)	0	0.1963(3)	0.0141(9)
S2	*4i*	0.6048(2)	0	0.0248(3)	0.0128(8)
S3	*4i*	0.8284(2)	0	0.1029(3)	0.0129(8)
S4	*4i*	0.4101(3)	0	0.3460(3)	0.0144(9)
S5	*4i*	0.2558(2)	0	0.7096(3)	0.0129(9)
S6	*4i*	0.3470(3)	0	0.5497(4)	0.0172(9)