Supporting Information File

Ternary Alkali ion Thiogallates, A_5GaS_4 (A = Li and Na) with Isolated Tetrahedral Building Units and Their Ionic conductivity

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Table S1. Final atomic coordinates and equivalent isotropic displacement parameters of the atoms for compounds **I** and **II**. $U_{(eq)}$ = 1/3rd of the trace of the orthogonalized U_{eq} tensor.

Atomic Parameters						
Atom	Wyckoff	Occupancy	x/a	y/b	z/c	U [Å^2]
Li_5GaS_4 (**I**)						
Ga1	2e	1	0.6335	0.25	0.1709	0.0166
S1	4f	1	0.7577	0.015	0.3271	0.0173
S2	2e	1	0.2704	0.25	0.1751	0.0159
S3	2e	1	2418	0.75	0.138	0.0167
Li1	4f	1	0.3577	0.5133	0.3341	0.0247
Li2	2e	1	0.0114	0.25	0.4846	0.0240
Li3	2e	1	0.649	0.75	0.1663	0.0280
Li4	2a	1	0	0	0	0.0420
Na_5GaS_4(**II**)						
Ga1	8c	1	0.4597	0.1673	0.3742	0.01148
S1	8c	1	0.13	0.7947	0.4575	0.0157
S2	8c	1	0.4452	0.8445	0.3782	0.0152
S3	8c	1	0.3574	0.7477	0.6238	0.0157
S4	8c	1	0.3696	0.261	0.2861	0.0163
Na1	8c	1	0.3508	0.9054	0.499	0.0261
Na2	8c	1	0.2852	0.55	0.3645	0.0197
Na3	8c	1	0.5553	0.5599	0.4342	0.0264
Na4	8c	1	0.4109	0.8763	0.2489	0.0272
Na5	8c	1	0.661	0.8877	0.3313	0.0234

Table S2. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

Atoms	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
			Li_5GaS_4 (**I**)			
Ga(1)	16(1)	15(1)	18(1)	0	0(1)	0
S(1)	18(1)	16(1)	18(1)	1(1)	-1(1)	1(1)
S(2)	14(1)	14(1)	19(1)	0	1(1)	0
S(3)	18(1)	15(1)	17(1)	0	1(1)	0
Li(1)	36(5)	20(4)	18(4)	-2(3)	-2(4)	3(3)
Li(2)	16(5)	23(6)	33(7)	0	-1(4)	0
Li(4)	25(6)	55(10)	45(9)	5(6)	13(6)	13(6)
Li(3)	48(8)	27(7)	10(5)	0	-3(5)	0
			Na_5GaS_4 (**II**)			
Ga(1)	8(1)	11(1)	11(1)	0(1)	0(1)	0(1)
S(1)	15(1)	16(1)	12(1)	-2(1)	-2(1)	-1(1)
S(2)	13(1)	11(1)	17(1)	1(1)	0(1)	0(1)
S(3)	9(1)	18(1)	16(1)	-1(1)	1(1)	-2(1)
S(4)	15(1)	17(1)	12(1)	2(1)	0(1)	2(1)
Na(1)	27(1)	28(1)	19(1)	5(1)	0(1)	-3(1)
Na(2)	14(1)	17(1)	24(1)	1(1)	-2(1)	2(1)
Na(3)	34(1)	18(1)	21(1)	-3(1)	-9(1)	6(1)
Na(4)	26(1)	33(1)	18(1)	-9(1)	-5(1)	8(1)
Na(5)	13(1)	29(1)	22(1)	-8(1)	-3(1)	5(1)

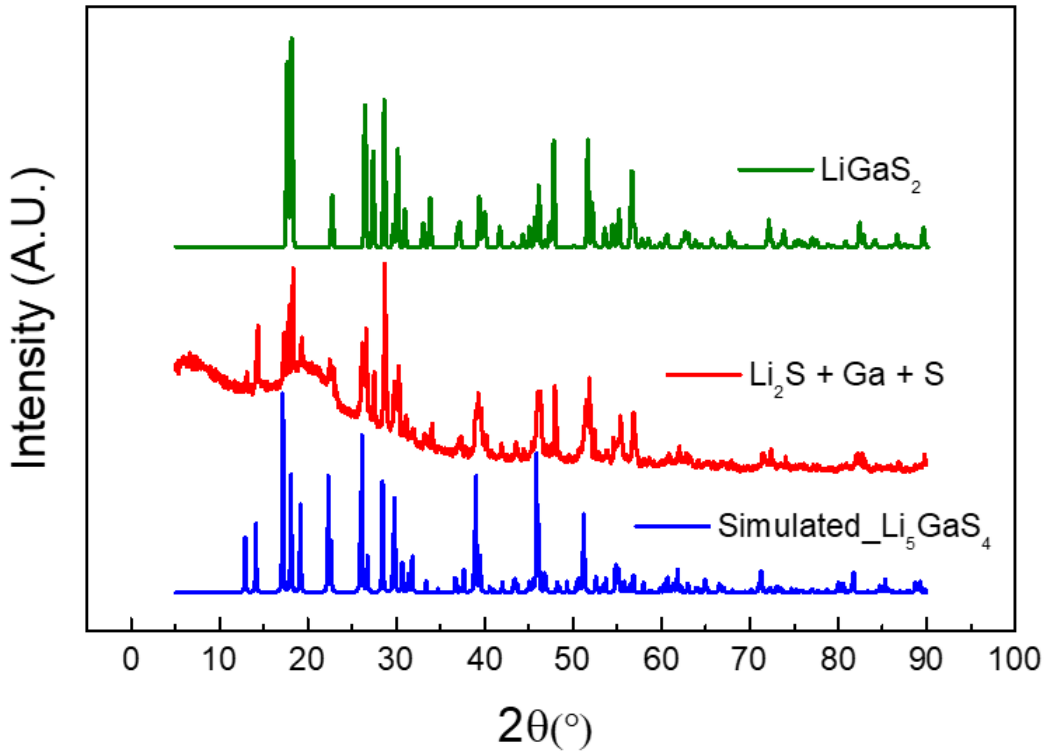


Figure S1: PXRD comparison of product from sealed tube reaction with simulated pattern of Li_5GaS_4 and the simulated pattern of the secondary phase $LiGaS_2$.

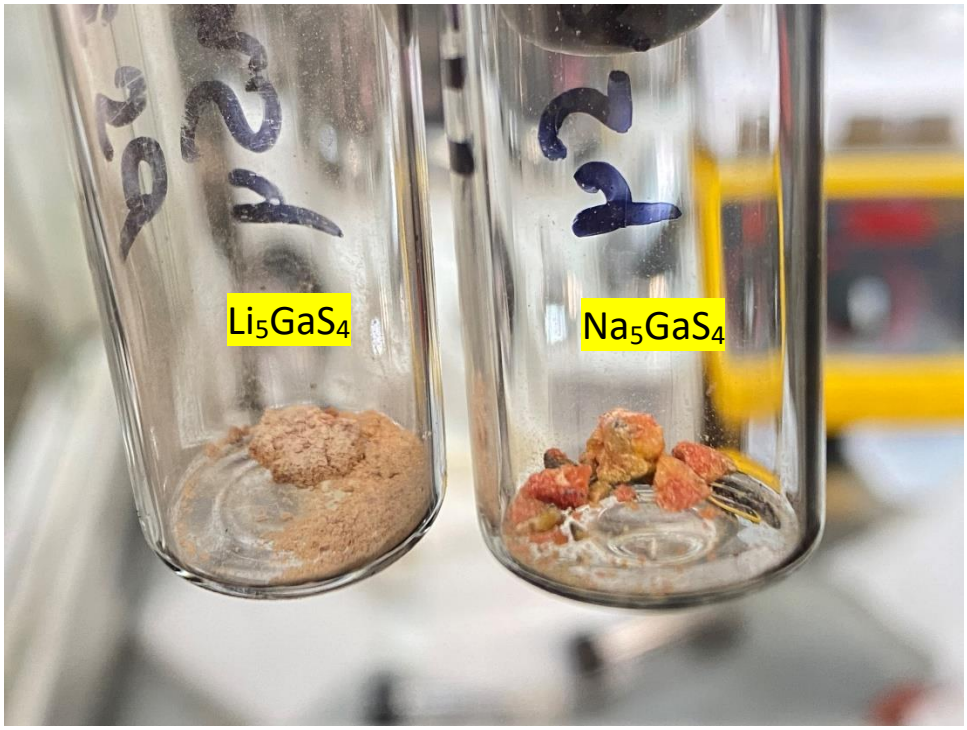


Figure S2: Photographs of the as synthesized crystals of compounds Li_5GaS_4 (**I**) and Na_5GaS_4 (**II**).

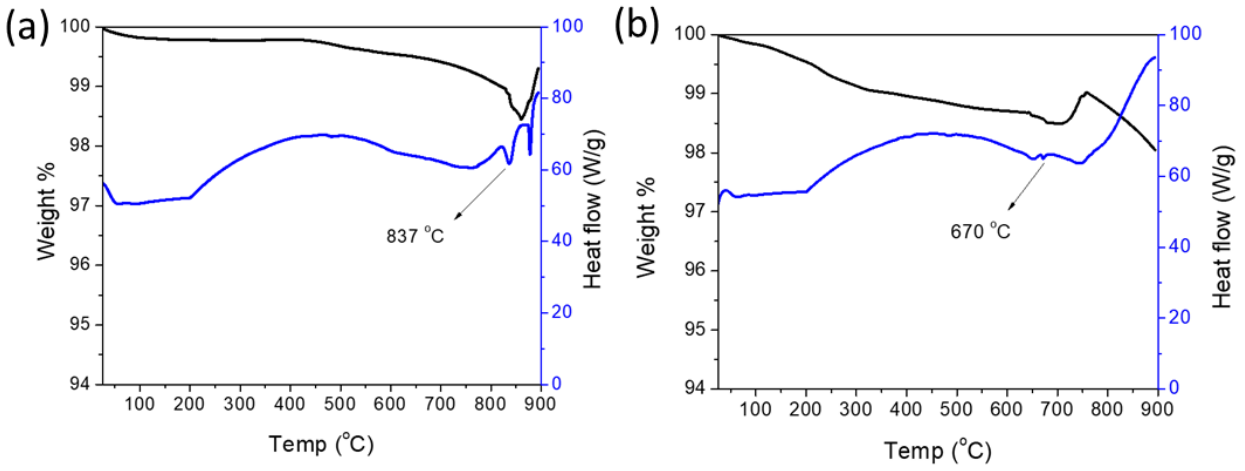


Figure S3: TGA and DSC plots of (a) compound **I**, Li_5GaS_4 and (b) compound **II**, Na_5GaS_4.

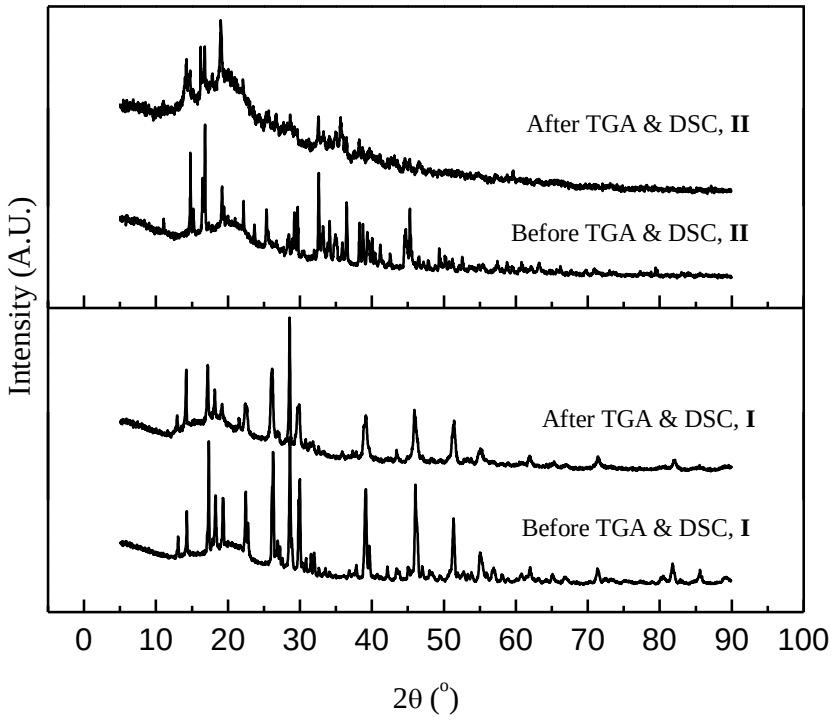


Figure S4: Comparison of PXRDs of **I** and **II** before and after simultaneous TGA & DSC.

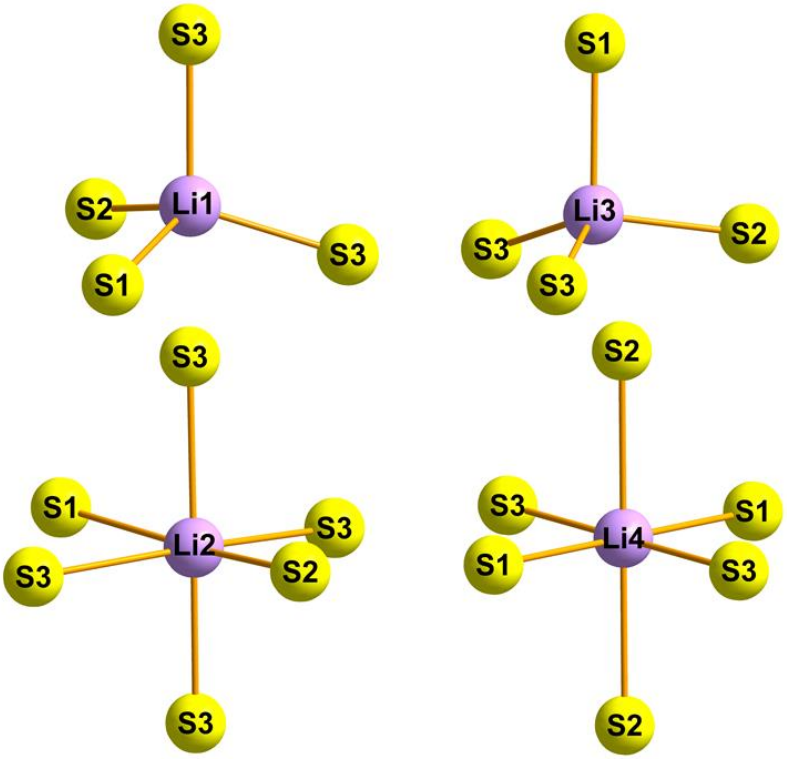


Figure S5: Coordination environment of Li atoms in Li_5GaS_4 (**I**).

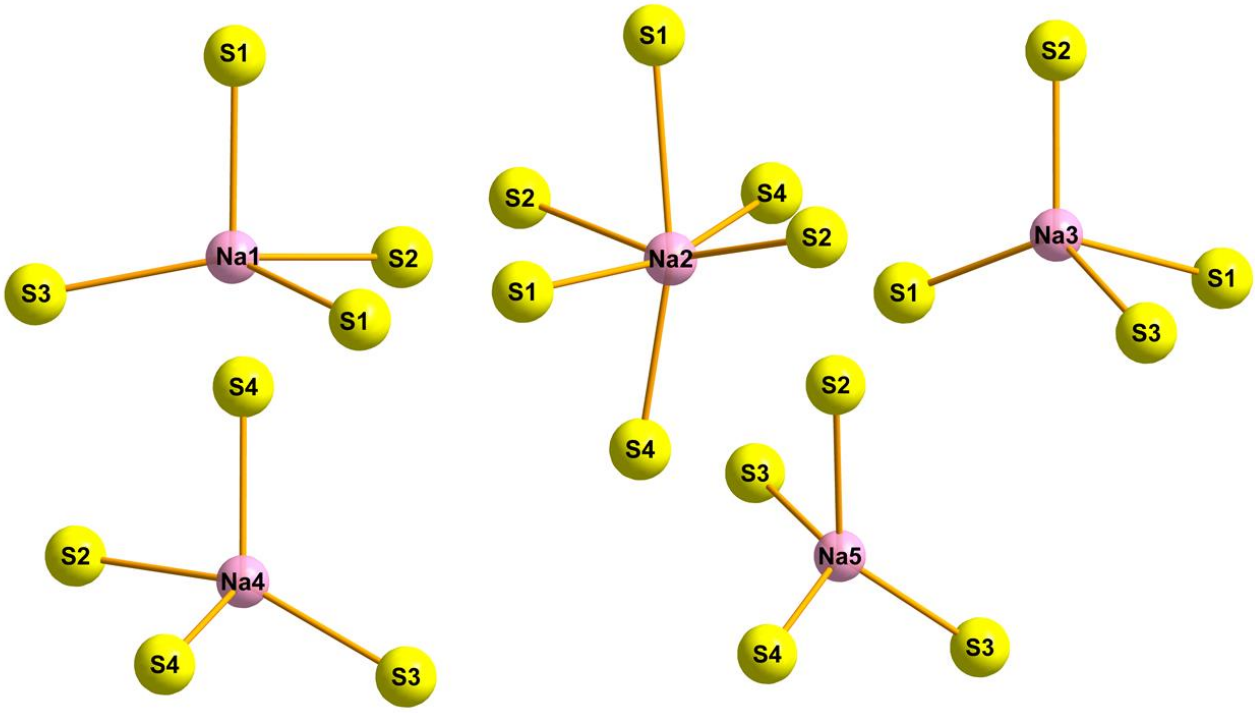
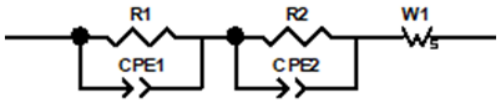


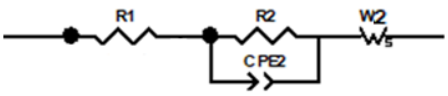
Figure S6: Coordination environment of Na atoms in Na_5GaS_4 (**II**).

Li_5GaS_4



R1 = 788 205 Ohm
Q1 = 14.3e-9 F.s^(a - 1)
a1 = 0.664 9
R2 = 1.616e6 Ohm
Q2 = 0.235 3e-9 F.s^(a - 1)
a2 = 0.797 9
s3 = 473 492 Ohm.s-^1/2

Na_5GaS_4



R1 = 7.803e-15 Ohm
R2 = 863 551 Ohm
Q2 = 78.22e-12 F.s^(a - 1)
a2 = 0.869 6
s2 = 1.697e6 Ohm.s-^1/2

Figure S7: Equivalent circuit and the parameters used to fit the impedance data for Li_5GaS_4 (**I**) and Na_5GaS_4 (**II**).