Electronic Supplementary Information (ESI)

Na_2GaS_2Cl: A New Sodium-Rich Chalcohalide with Two-Dimensional $[GaS_2]_\infty$ Layers and Wide Interlayer Space

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†Electronic supplementary information (ESI) available: Coordination environments of all cations, atomic coordinates, isotropic displacement parameters. CCDC 2073426. For ESI and crystallographic data in CIF or other electronic format see DOI: XXX.

1. Tables and Figures

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Figure S1. The thermal vibration ellipsoids of all atoms in Na_2GaS_2Cl.

Figure S2. Coordination environments of all cations in Na_2GaS_2Cl.

Figure S3. (a) Band structure of $NaGaS_2$. (b) The total and partial density of states (DOS and PDOS, respectively) of $NaGaS_2$. Dashed line represents the Fermi energy (E_f).

Table S1. Fractional atomic coordinates, equivalent isotropic displacement parameters, and bond valence sums (BVS) for Na_2GaS_2Cl. U_{eq} is defined as 1/3 of of the trace of the orthogonalized U_{ij} tensor.

Atom	Wyck.	S.O.F.	x/*a*	y/*b*	z/*c*	U_{eq} [Å^2]	BVS
Na1	4a	1	1/2	1/2	1/2	0.0161(11)	1.072
Na2	4c	1	1/2	0.16772(13)	1/4	0.0205(12)	0.972
Na3	4c	1	1/2	0.16675(16)	3/4	0.0277(14)	0.894
Na4	4c	1	1.00000	0.41771(14)	3/4	0.0211(12)	0.948
Na5	4c	1	1/2	0.41675(14)	3/4	0.0224(12)	0.890
Na6	4b	1	1.00000	1/2	1.00000	0.0131(10)	1.052
Na7	8g	1	0.2486(5)	0.24980(8)	1/4	0.0166(9)	1.010
Ga1	8f	1	1/2	0.34152(2)	0.49611(11)	0.0093(3)	2.985
Ga2	8g	1	0.74645(10)	0.40851(2)	1/4	0.0083(3)	2.917
S1	4c	1	1/2	0.30624(7)	1/4	0.0110(6)	-1.940
S2	4c	1	1/2	0.30793(8)	3/4	0.0132(6)	-1.890
S3	16h	1	0.75619(17)	0.37464(6)	0.50611(17)	0.0112(3)	-1.854
S4	4c	1	1.00000	0.44265(7)	1/4	0.0101(6)	-1.854
S5	4c	1	1/2	0.44337(8)	1/4	0.0105(6)	-1.976
Cl1	8f	1	1/2	0.22045(5)	0.5000(3)	0.0128(4)	-1.023
Cl2	8g	1	0.7502(3)	0.47044(5)	3/4	0.0117(4)	-1.020

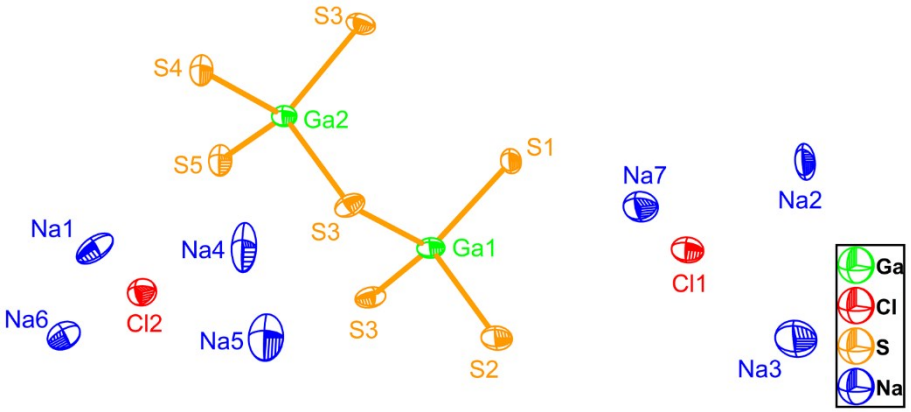

Figure S1. The thermal vibration ellipsoids of all atoms in Na_2GaS_2Cl.

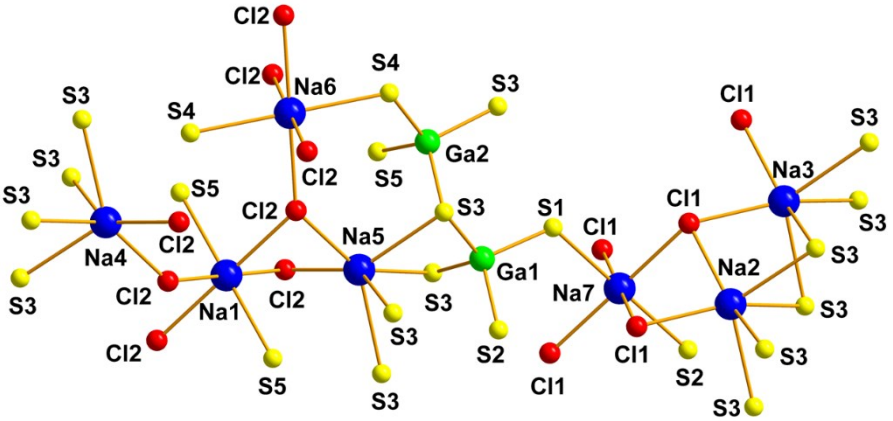

Figure S2. Coordination environments of all cations in Na_2GaS_2Cl.

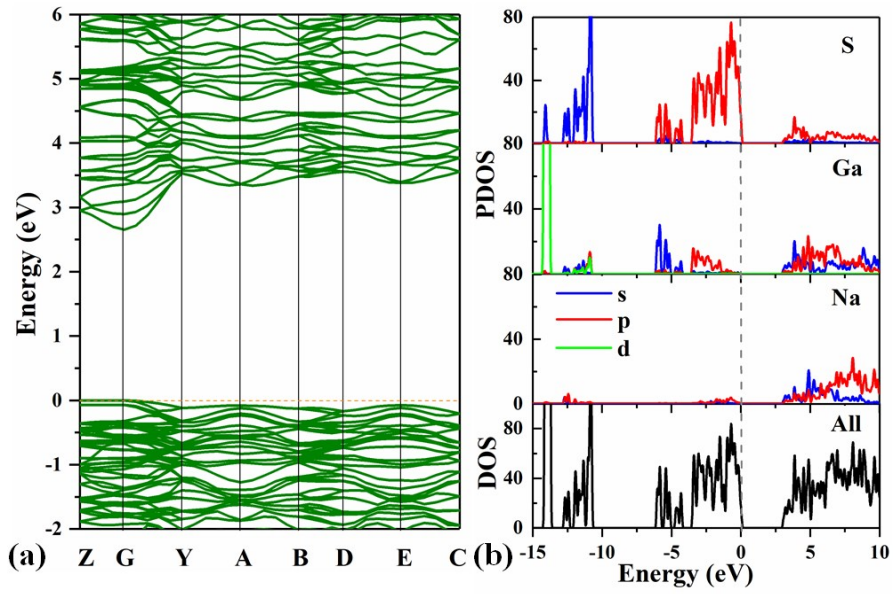

Figure S3. (a) Band structure of $NaGaS_2$. (b) The total and partial density of states (DOS and PDOS, respectively) of $NaGaS_2$. Dashed line represents the Fermi energy (E_f).