Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

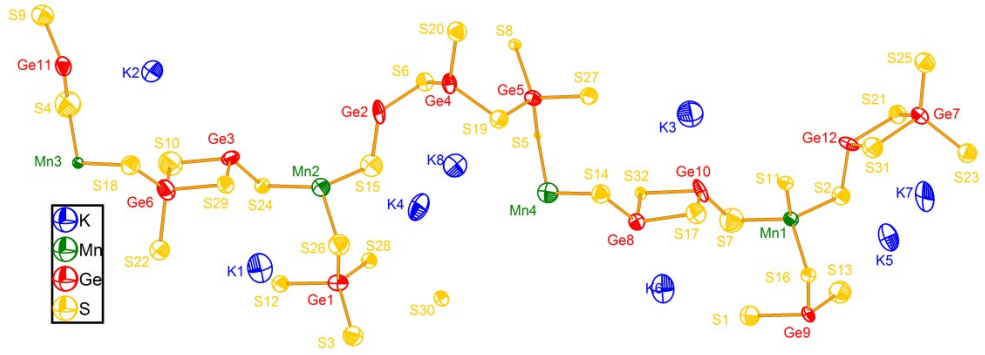

Figure S1. asymmetric unit of $K_2MnGe_3S_8$

Table S1 Atomic coordinates($\times 10^4$) and equivalent isotropic displacement parameters in $Å^2 \times 10^3$ of $K_2MnGe_3S_8$

Atom	Oxidation	Wyckoff	*x*	*y*	*z*	U_{eq}
K1	+1	2*a*	8038(4)	9126.1(18)	5390.8(7)	31.7(6)
K2	+1	2*a*	−1568(3)	5701.5(19)	5964.0(6)	26.4(6)
K3	+1	2*a*	3027(3)	9062(2)	394.2(7)	34.7(3)
K4	+1	2*a*	6161(3)	8673(2)	3520.8(7)	30.9(6)
K5	+1	2*a*	11094(3)	8656.9(18)	–1476.7(6)	25.1(6)
K6	+1	2*a*	13481(3)	5673.4(18)	954.6(6)	28.6(6)
K7	+1	2*a*	10651(3)	5341.0(18)	–2094.3(6)	28.7(6)
K8	+1	2*a*	5685(3)	5335(2)	2900.4(7)	32.1(6)
Mn1	+2	2*a*	10113.2(17)	7105.9(10)	–530.0(4)	11.1(2)

Mn2	+2	2*a*	5115.4(19)	7109.7(12)	4467.9(4)	17.7(2)
Mn3	+2	2*a*	2047.8(16)	7221.4(9)	7034.5(3)	6.6(2)
Mn4	+2	2*a*	6981(2)	7171	2033.2(4)	22.2(3)
Ge1	+4	2*a*	10104.5(12)	7430.7(7)	4515.2(3)	12.7(2)
Ge2	+4	2*a*	1817.3(14)	6529.6(8)	3645.4(3)	15.5(2)
Ge3	+4	2*a*	3076.9(12)	6752.3(8)	5360.0(3)	15.2(2)
Ge4	+4	2*a*	364.2(13)	7604.9(8)	2864.0(3)	13.5(2)
Ge5	+4	2*a*	2000.7(12)	6932.7(8)	1965.4(3)	12.25(18)
Ge6	+4	2*a*	3819.4(14)	7869.5(8)	6172.7(3)	19.0(3)
Ge7	+4	2*a*	5384.6(13)	7609.0(9)	–2136.5(3)	16.7(3)
Ge8	+4	2*a*	8831.4(13)	7885.4(8)	1170.5(3)	12.12(18)
Ge9	+4	2*a*	15112.3(13)	7406.3(8)	–486.1(3)	14.1(2)
Ge10	+4	2*a*	8142.1(14)	6754.5(8)	365.2(3)	15.5(2)
Ge11	+4	2*a*	–3005.0(13)	6944.6(8)	6959.9(3)	15.5(2)
Ge12	+4	2*a*	6826.8(13)	6518.3(8)	–1351.6(3)	14.3(2)
S1	–2	2*a*	15150(3)	6528(2)	110.8(7)	20.2(3)
S2	–2	2*a*	9693(3)	6092.5(19)	–1162.6(6)	16.4(3)
S3	–2	2*a*	12571(3)	8407(2)	4514.2(7)	20.4(3)
S4	–2	2*a*	–519(4)	5888(3)	6955.9(8)	34.4(3)
S5	–2	2*a*	4459(2)	5899.3(15)	1964.3(5)	1.8(3)
S6	–2	2*a*	881(3)	5799.9(19)	3053.3(6)	16.0(3)
S7	–2	2*a*	10245(4)	5998(2)	68.1(7)	29.6(3)

S8	–2	2*a*	–474(3)	5886.9(17)	1999.0(5)	6.8(3)
S9	–2	2*a*	–5375(3)	5919(2)	7024.9(7)	25.2(3)
S10	–2	2*a*	3235(4)	6083(2)	5991.5(8)	29.9(3)
S11	–2	2*a*	7601(3)	8443.8(18)	–502.5(6)	10.6(3)
S12	–2	2*a*	10157(3)	6480.6(19)	5101.6(6)	14.5(3)
S13	–2	2*a*	14780(3)	6004(2)	–934.6(7)	24.6(3)
S14	–2	2*a*	6782(3)	8638.0(19)	1525.1(6)	17.4(3)
S15	–2	2*a*	4746(4)	6134(2)	3833.8(7)	24.7(3)
S16	–2	2*a*	12589(3)	8476.6(18)	–534.0(6)	10.7(3)
S17	–2	2*a*	8509(3)	8579(2)	540.5(7)	20.7(3)
S18	–2	2*a*	1928(3)	8642(2)	6530.9(7)	18.3(3)
S19	–2	2*a*	2283(3)	8270.5(19)	2436.8(6)	16.6(3)
S20	–2	2*a*	–2535(3)	8107.6(19)	2684.7(7)	18.9(3)
S21	–2	2*a*	5926(3)	5838(2)	–1970.7(7)	16.6(3)
S22	–2	2*a*	6882(3)	7977(2)	6384.9(7)	20.3(3)
S23	–2	2*a*	7407(3)	8229.8(19)	–2537.8(7)	18.0(3)
S24	–2	2*a*	5155(3)	5872.9(18)	5044.7(6)	11.2(3)
S25	–2	2*a*	2464(3)	7976(2)	–2297.1(7)	19.9(3)
S26	–2	2*a*	7664(3)	8466(2)	4458.5(7)	22.1(3)
S27	–2	2*a*	1824(3)	8015.8(19)	1401.9(6)	15.2(3)
S28	–2	2*a*	9771(3)	6004.4(18)	4071.3(6)	11.8(3)
S29	–2	2*a*	3670(3)	8533.0(19)	5547.3(6)	14.9(3)

S30	–2	2*a*	11276(3)	8318.4(18)	3472.0(6)	11.1(3)
S31	–2	2*a*	6396(3)	8340(2)	–1524.8(7)	20.9(3)
S32	–2	2*a*	8141(3)	6082.0(16)	987.9(5)	6.8(3)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.