

Supplementary Materials

$A\text{Ag}_3\text{Ga}_8\text{Se}_{14}$ (A = Rb, Cs): Second-Harmonic Generation Responses Realized through the Parallel Arrangement of AgSe_4 and GaSe_4 Tetrahedrons

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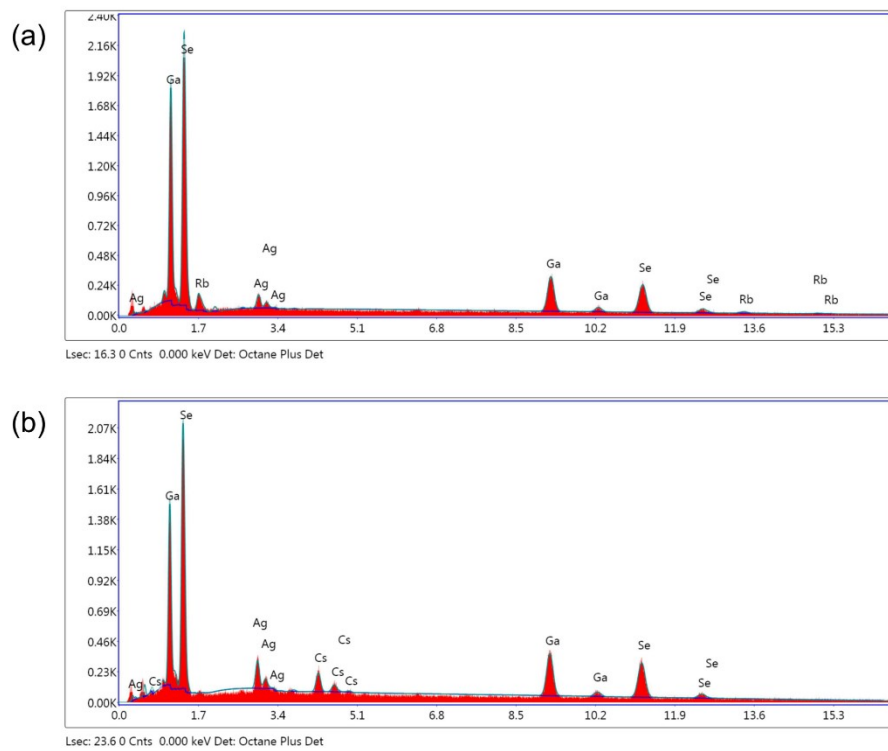


Fig. S1 EDS spectra of $\text{RbAg}_3\text{Ga}_8\text{Se}_{14}$ (**1**, a) and $\text{CsAg}_3\text{Ga}_8\text{Se}_{14}$ (**2**, b).

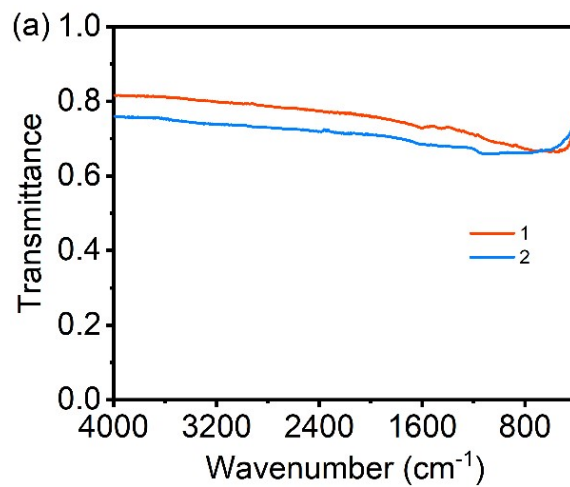


Fig. S2 IR spectra of **1** and **2**.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1** and **2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Compound 1				
Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Rb1	6139.5(19)	10000	4239(3)	39.2(5)
Ag1	9954.7(10)	10000	7189.8(14)	24.1(3)
Ag2	2019.3(10)	10000	5173.6(14)	22.1(3)
Ag3	7811.2(10)	10000	9617.2(14)	22.2(3)
Ga1	7952.6(8)	6714.1(10)	9447.6(11)	8.1(3)
Ga2	5015.7(9)	8297.3(8)	7407.5(12)	7.7(2)
Ga3	5927.7(8)	6650.2(10)	1441.0(11)	8.1(2)
Ga4	8994.6(9)	8358.3(9)	3501.1(13)	8.2(2)
Se1	9993.8(8)	6643.9(8)	9951.9(10)	6.6(2)
Se2	10000.1(12)	10000	10000.0(15)	9.7(3)
Se3	7979.7(7)	6636.3(8)	1976.3(9)	6.7(2)
Se4	2172.6(12)	10000	8049.5(14)	9.9(3)
Se5	5938.7(8)	6912.6(9)	3887.7(11)	8.7(2)
Se6	6973.2(8)	8240.6(10)	7789.5(10)	8.9(2)
Se7	8795.7(8)	8190.3(9)	5838.4(10)	8.3(2)
Se8	7840.4(11)	10000	2298.8(15)	9.2(3)
Se9	4255.6(11)	10000	5927.8(15)	8.3(3)
Compound 2				
Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Cs1	3948.9(10)	0	5890.3(13)	29.1(3)
Ag1	49.6(11)	0	2826.2(16)	27.6(3)
Ag2	7991.3(11)	0	4782.5(15)	24.6(3)
Ag3	2166.8(10)	0	424.0(15)	25.1(3)
Ga1	2045.1(9)	3283.4(9)	538.7(12)	10.9(3)
Ga2	4984.4(10)	1704.9(8)	2580.6(14)	11.0(3)
Ga3	4065.9(9)	3358.1(10)	8548.4(11)	11.5(3)
Ga4	994.2(10)	1632.9(10)	6499.7(14)	10.9(3)
Se1	5.9(8)	3338.6(8)	38.1(11)	10.0(2)
Se2	-18.2(12)	0	9.8(16)	13.1(3)
Se3	2015.4(8)	3352.9(7)	8012.9(10)	9.9(2)
Se4	7825.8(11)	0	1919.4(14)	12.9(3)
Se5	4052.0(8)	3109.6(8)	6105.6(11)	11.8(2)
Se6	3033.5(8)	1769.7(10)	2207.4(10)	12.0(2)
Se7	1196.4(8)	1811.4(8)	4166.4(11)	11.6(2)
Se8	2129.3(11)	0	7736.6(15)	12.6(3)
Se9	5764.9(12)	0	4019.6(15)	11.1(3)

Table S2. Selected bond lengths for **1** and **2**.

Compound 1			
Bond	Length/Å	Bond	Length/Å
Rb1–Se8	3.4650(2)	Ag3–Se2	2.6832(7)
Rb1–Se9	3.4810(2)	Ga1–Se6	2.3620(6)
Rb1–Se5×2	3.6382(1)	Ga1–Se4	2.3834(3)
Rb1–Se6×2	3.7320(2)	Ga1–Se3	2.4314(5)
Rb1–Se7×2	3.7360(2)	Ga1–Se1	2.4603(2)
Rb1–Se3×2	4.1470(2)	Ga2–Se6	2.3882(4)
Rb1–Se1×2	4.2010(1)	Ga2–Se7	2.3896(4)
Ag1–Se7	2.5928(2)	Ga2–Se9	2.3995(2)
Ag1–Se7	2.5928(2)	Ga2–Se1	2.4739(4)
Ag1–Se4	2.6042(8)	Ga3–Se2	2.3760(3)
Ag1–Se2	2.6920(2)	Ga3–Se5	2.3795(4)
Ag2–Se5	2.6443(1)	Ga3–Se1	2.4485(6)
Ag2–Se5	2.6443(1)	Ga3–Se3	2.4645(3)
Ag2–Se9	2.6463(6)	Ga4–Se5	2.3900(4)
Ag2–Se4	2.6986(7)	Ga4–Se7	2.3933(4)
Ag3–Se8	2.5764(6)	Ga4–Se8	2.3974(3)
Ag3–Se6	2.6192(3)	Ga4–Se3	2.5022(4)
Ag3–Se6	2.6193(3)		

Compound 2			
Bond	Length/Å	Bond	Length/Å
Cs1–Se8	3.5482(7)	Ag3–Se2	2.6768(7)
Cs1–Se9	3.5632(8)	Ga1–Se6	2.3620(7)
Cs1–Se5×2	3.6721(9)	Ga1–Se4	2.3862(3)
Cs1–Se6×2	3.8347(4)	Ga1–Se3	2.4346(7)
Cs1–Se7×2	3.8366(3)	Ga1–Se1	2.4651(3)
Cs1–Se3×2	4.0552(4)	Ga2–Se6	2.3901(6)
Cs1–Se1×2	4.1151(6)	Ga2–Se7	2.3912(5)
Ag1–Se7	2.5927(1)	Ga2–Se9	2.3962(3)
Ag1–Se7	2.5927(1)	Ga2–Se1	2.4797(5)
Ag1–Se4	2.6085(8)	Ga3–Se2	2.3772(3)
Ag1–Se2	2.6940(2)	Ga3–Se5	2.3798(4)
Ag2–Se5	2.6301(1)	Ga3–Se1	2.4474(7)
Ag2–Se5	2.6301(1)	Ga3–Se3	2.4690(4)
Ag2–Se9	2.6378(7)	Ga4–Se5	2.3906(4)
Ag2–Se4	2.6876(8)	Ga4–Se8	2.3921(5)
Ag3–Se8	2.5855(9)	Ga4–Se7	2.4025(5)
Ag3–Se6	2.6189(3)	Ga4–Se3	2.5040(6)
Ag3–Se6	2.6189(3)		