

Supporting Information (SI)

Open Honeycomb Frameworks of Sulphides $A\text{Hg}_4\text{Ga}_5\text{S}_{12}$ (A = Rb, Cs)

Exhibiting Infrared Nonlinear Optical Properties

Xiao-Yu Lou, ^{a,b} Yu Zhou, ^{a,b} Wen-Fa Chen, ^b Xiao-Ming Jiang, ^b Bin-Wen Liu, ^{b,*}
and Guo-Cong Guo ^{b,*}

^a *Fuzhou University, Fuzhou, Fujian 350108, People's Republic of China*

^b *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China*

E-mails: bwliu@fjirsm.ac.cn (B.-W. Liu), gcguo@fjirsm.ac.cn (G.-C. Guo)

Contents

Figures and Tables

Fig. S1 EDS results.

Fig.S2 The experimental and calculated powder XRD results of Le Bail Profile fitting procedures.

Fig. S3 IR spectra.

Fig. S4 Calculated refractive indexes.

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters.

Table S2. Selected bond distances (Å).

Table S3. Bond Angles (°).

Figures and Tables

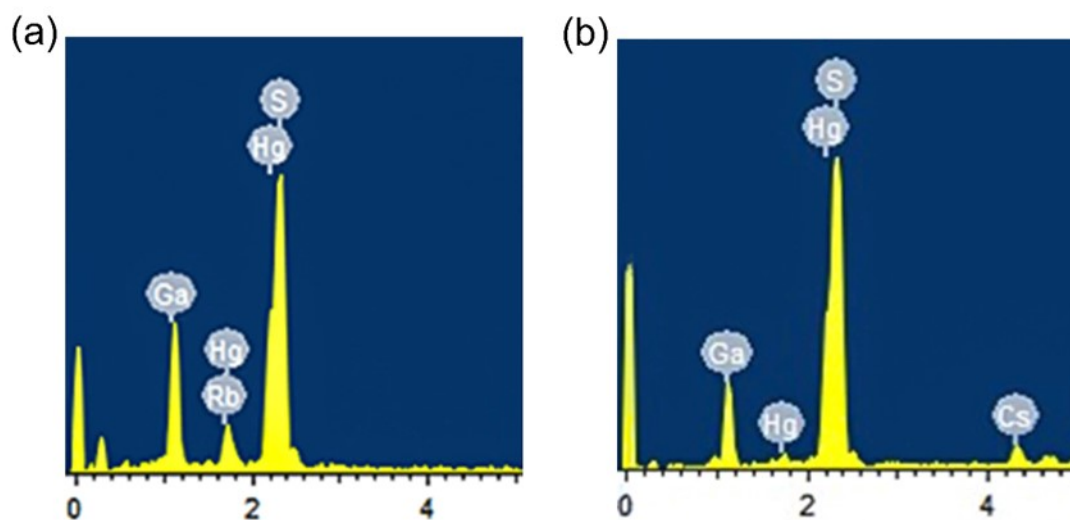


Fig. S1 EDS results of **1**(a) and **2**(b).

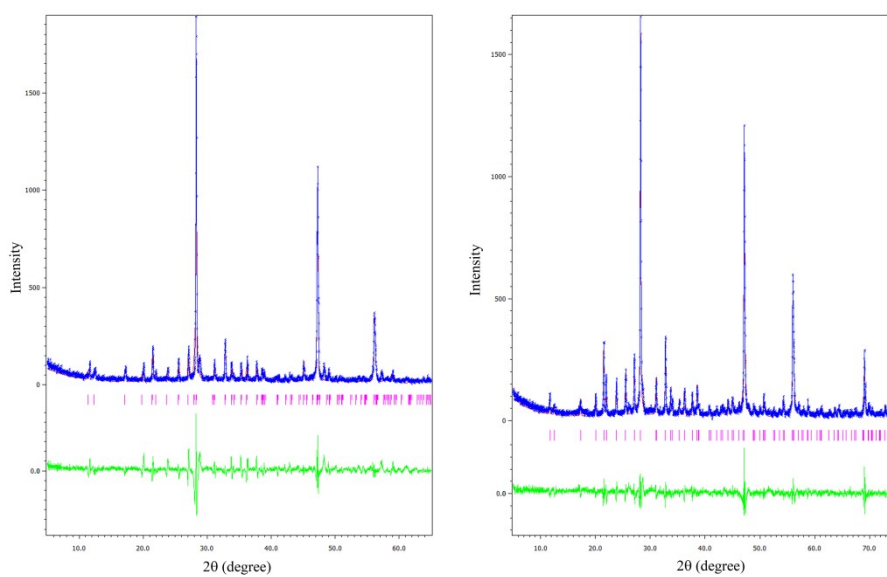


Fig. S2 The experimental (blue line) and calculated (red line) powder XRD results of Le Bail Profile fitting procedures for **1** and **2**, respectively.

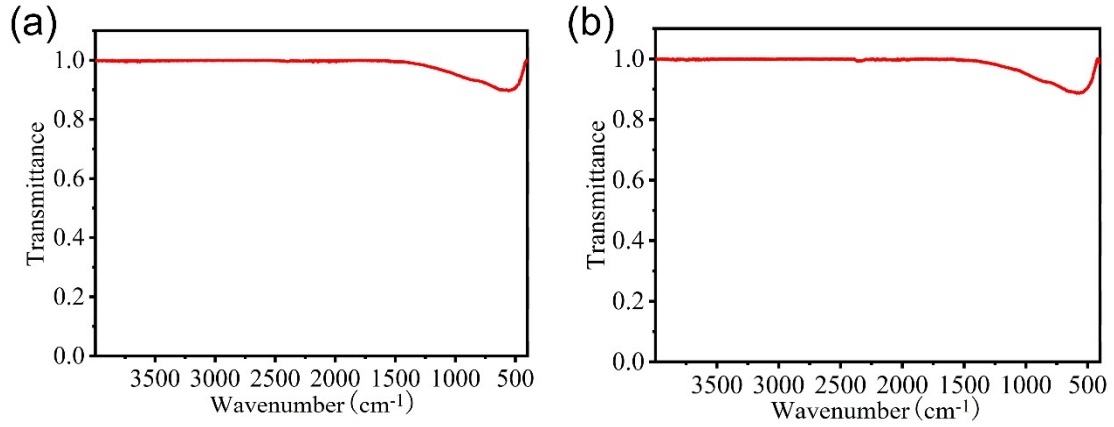


Fig. S3 IR spectra of 1(a) and 2(b).

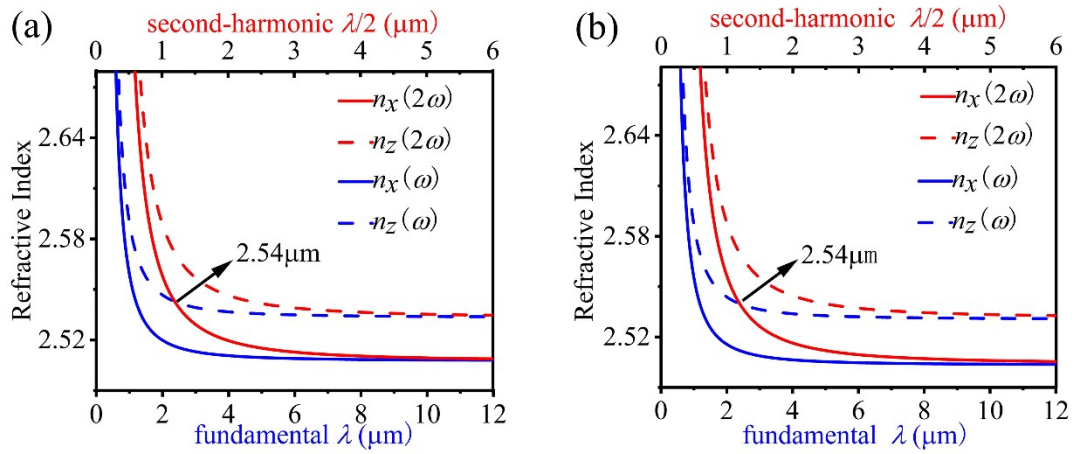


Fig. S4 Calculated refractive indexes of 1 (a) and 2 (b).

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1** and **2**.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
1				
Rb1	10000	0	6973(4)	36.1(7)
Hg/Ga (1)	10256(3)	4349(4)	1110.9(1)	22.3(6)
Hg/Ga (2)	9476(1)	1283(1)	1179(1)	22.9(4)
Hg/Ga (3)	6467(3)	-967(3)	1115.6(4)	24.2(7)
S1	5032(3)	-2846(3)	391(7)	23.4(12)
S2	6325(4)	-1084(5)	3666(8)	36.5(15)
S3	7172(3)	2069(3)	3446(7)	28.3(14)
S4	10340(4)	4446(4)	3629(7)	26.6(12)
2				
Cs1	10000	10000	39(2)	22.5(4)
Hg/Ga (1)	7950(2)	5136(6)	9177(5)	27.3(5)
Hg/Ga (2)	4104(3)	9798(3)	9220(5)	22.9(9)
Hg/Ga (3)	6419(2)	8987(3)	9244(1)	21.4(6)
S1	9230(4)	7005(5)	54(1)	30.1(2)
S2	4548(4)	8374(4)	9953(6)	24.1(12)
S3	7002(5)	7750(7)	1001(1)	38.3(2)
S4	6160(5)	4607(5)	204(5)	32.0(14)

Table S2. Selected bond distances (\AA) for **1** and **2**.

Bond	Distance/ \AA	Bond	Distance / \AA
1			
Rb (1)–S (1) \times 3	3.685(5)	Hg/Ga (2)–S (1) \times 3	2.382(7)
Rb (1)–S (2) \times 3	3.720(5)	Hg/Ga (3)–S (3) \times 3	2.376(6)
Rb (1)–S (3) \times 3	3.655(5)	Hg/Ga (2)–S (3) \times 3	2.407(4)
Rb (1)–S (4) \times 3	3.711(5)	Hg/Ga (2)–S (3) \times 3	2.423(5)
Hg/Ga (1)–S (1) \times 3	2.369(6)	Hg/Ga (2)–S (4) \times 3	2.424(6)
Hg/Ga (1)–S (2) \times 3	2.346(8)	Hg/Ga (3)–S (2) \times 3	2.388(9)
Hg/Ga (1)–S (4) \times 3	2.359(6)	Hg/Ga (1)–S (4) \times 3	2.359(6)
Hg/Ga (1)–S (4) \times 3	2.357(7)	Hg/Ga (2)–S (4) \times 3	2.424(6)
2			
Cs (1)–S (1) \times 3	3.736(7)	Hg/Ga (2)–S (2) \times 3	2.439(7)
Cs (1)–S (2) \times 3	3.708(4)	Hg/Ga (2)–S (3) \times 3	2.402(11)
Cs (1)–S (3) \times 3	3.741(7)	Hg/Ga (2)–S (4) \times 3	2.369(7)
Cs (1)–S (4) \times 3	3.697(5)	Hg/Ga (3)–S (1) \times 3	2.356(6)
Hg/Ga (1)–S (1) \times 3	2.429(7)	Hg/Ga (3)–S (1) \times 3	2.372(6)
Hg/Ga (1)–S (2) \times 3	2.404(5)	Hg/Ga (3)–S (2) \times 3	2.382(7)

Hg/Ga (1)–S (4) × 3	2.408(5)	Hg/Ga (3)–S (3) × 3	2.341(9)
Hg/Ga (1)–S (4) × 3	2.420(7)	Hg/Ga (1)–S (2) × 3	2.404(5)

Table S3. Bond Angles (°) for **1** and **2**.

Bond Angles	Angle/°	Bond Angles	Angle/°
1			
∠S(2)-(Hg/Ga)1-S(1)	111.3(3)	∠S(3)-(Hg/Ga)2-S(3)	102.7(2)
∠S(1)-(Hg/Ga)1-S(4)	107.1(3)	∠S(3)-(Hg/Ga)2-S(4)	106.08(19)
∠S(2)-(Hg/Ga)1-S(4)	105.7(2)	∠S(3)-(Hg/Ga)2-S(4)	108.8(2)
∠S(4)-(Hg/Ga)1-S(1)	104.4(2)	∠S(4)-(Hg/Ga)3-S(3)	109.9(2)
∠S(4)-(Hg/Ga)1-S(1)	116.2(3)	∠S(2)-(Hg/Ga)3-S(1)	102.1(2)
∠S(4)-(Hg/Ga)1-S(4)	111.9(3)	∠S(2)-(Hg/Ga)3-S(2)	108.1(2)
∠S(1)-(Hg/Ga)2-S(3)	112.92(18)	∠S(3)-(Hg/Ga)3-S(1)	110.7(3)
∠S(1)-(Hg/Ga)2-S(3)	112.49(16)	∠S(3)-(Hg/Ga)3-S(2)	116.7(2)
∠S(1)-(Hg/Ga)2-S(4)	113.12(19)	∠S(3)-(Hg/Ga)3-S(2)	110.0(2)
Bond Angles	Angle/°	Bond Angles	Angle/°
2			
∠S(2)-(Hg/Ga)1-S(1) × 2	112.67(18)	∠S(4)-(Hg/Ga)2-S(2)	110.7(3)
∠S(2)-(Hg/Ga)1-S(4)	112.10(15)	∠S(4)-(Hg/Ga)2-S(3)	116.3(2)
∠S(2)-(Hg/Ga)1-S(4)	112.19(16)	∠S(4)-(Hg/Ga)2-S(3)	109.9(2)
∠S(4)-(Hg/Ga)1-S(1)	109.0(2)	∠S(1)-(Hg/Ga)3-S(1)	111.7(3)
∠S(4)-(Hg/Ga)1-S(1)	106.27(17)	∠S(1)-(Hg/Ga)3-S(2)	115.8(3)
∠S(4)-(Hg/Ga)1-S(4)	104.1(2)	∠S(1)-(Hg/Ga)3-S(2)	104.1(2)
∠S(3)-(Hg/Ga)2-S(2)	102.6(2)	∠S(3)-(Hg/Ga)3-S(1)	107.1(3)
∠S(3)-(Hg/Ga)2-S(2)	108.7(3)	∠S(3)-(Hg/Ga)3-S(1)	106.5(17)
∠S(3)-(Hg/Ga)2-S(3)	108.2(2)	∠S(3)-(Hg/Ga)3-S(2)	111.4(3)

