Supporting Information for

Syntheses, structures, and properties of sulfides constructed by SbS_4 teeter-totter polyhedron: $Ba_3La_4Ga_2Sb_2S_{15}$ and $BaLa_3GaSb_2S_{10}$

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters of compound **1** and **2**.

Atom	Wyckoff	*x*	*y*	*z*	*U(eq)*
La1	8*j*	0.05421(4)	0.3355(2)	1/2	0.0132(3)
La2	8*j*	0.28521(4)	0.3660(2)	0.0000	0.0112(3)
Ba1	4*a*	0.0000	0.0000	1/4	0.0146(3)
Ba2	8*f*	0.16341(4)	1/2	3/4	0.0142(3)
Sb1	8*j*	0.10175(6)	0.7872(2)	1/2	0.0316(4)
Ga1	8*f*	0.17035(6)	0.0000	1/4	0.0093(4)
S1	16*k*	0.1183(2)	0.1624(3)	0.3514(2)	0.0135(5)
S2	8*j*	0.1671(2)	0.5021(4)	1/2	0.0137(8)
S3	16*k*	0.2240(2)	0.1506(3)	0.1435(2)	0.0142(5)
S4	16*k*	0.0493(2)	0.6465(3)	0.6317(2)	0.0136(5)
S5	*4c*	0.0000	1.0000	1/2	0.0174(2)

Atom	Wyckoff	*x*	*y*	*z*	*U(eq)*
La1	2*e*	0.6161(2)	1/4	0.05695(6)	0.0090(2)
La2	2*e*	1.1157(2)	1/4	0.94309(6)	0.0088(2)
La3	2*e*	1.8804(2)	1/4	0.69118(6)	0.0101(2)
La4	2*e*	1.38044(2)	1/4	0.30897(6)	0.0097(2)
La5	4*f*	1.24990(9)	-0.00004(6)	1.12751(4)	0.0145(2)
Ba1	4*f*	2.24990(9)	-0.00003(6)	0.61748(4)	0.61748(4)
Ga1	4*f*	0.7501(2)	-0.0001(4)	0.12602(7)	0.0084(3)
Sb1	2*e*	0.9526(2)	1/4	0.21986(7)	0.0138(3)
Sb2	2*e*	1.5277 (2)	1/4	0.53715(7)	0.0139(3)
Sb3	2*e*	2.0278(2)	1/4	0.46281(7)	0.0137(3)
Sb4	2*e*	1.4524(2)	1/4	0.78022(7)	0.0141(3)
S1	4*f*	1.5975(4)	0.1085(2)	0.7132(2)	0.0132(6)
S2	2*e*	0.7471(5)	1/4	-0.1220(2)	0.019(2)
S3	4*f*	1.0975(4)	0.1077(2)	0.2870(2)	0.0142(6)
S4	2*e*	0.2476(5)	1/4	0.1212(3)	0.020(2)
S5	4*f*	0.9029(4)	0.1028(2)	0.0380(2)	0.0133(6)
S6	4*f*	1.0760(4)	0.1030(2)	0.8004(2)	0.0120(6)
S7	4*f*	0.5763(4)	0.1028(2)	0.1028(2)	0.0119(6)
S8	4*f*	0.4021(4)	0.1018(2)	-0.0381 (2)	0.0128(6)
S9	4*f*	1.9136(4)	0.1126(2)	0.5474 (2)	0.0134(6)
S10	4*f*	0.0134(6)	0.1121(2)	0.4525(2)	0.0147(6)
S11	2*e*	2.2639(5)	1/4	0.6346(3)	0.0183(9)
S12	2*e*	1.7643(5)	1/4	0.3656(3)	0.0170(9)

Table S2. Selected bond lengths (Å) of compound **1** and **2**.

1					
La1–S1×2	2.870(3)	Ba1–S1×4	3.370(3)	Sb1–S4×2	2.443(3)
La1–S5	2.9398(9)	Ba1–S5×2	3.3976(2)	Sb1–S2	2.727(4)
La1–S2	2.972(4)	Ba1–S4×4	3.422(3)	Sb1–S5	2.932(2)
La1–S4×2	3.035(3)	Ba2–S1×2	3.182(3)	Ga1–S1×2	2.247(3)
La1–S4×2	3.039(3)	Ba2–S3×2	3.254(3)	Ga1–S3×2	2.261(3)
La2–S3×2	2.964(3)	Ba2–S4×2	3.345(3)		
La2–S2	2.979(4)	Ba2–S2×2	3.3988(2)		
La2–S3×2	2.982(3)	Ba2–S3×2	3.425(3)		
La2–S1×2	3.054(3)				
La2–S2	3.114(4)				

2					
La1–S2	2.940(4)	La5–S6	3.091(3)	Ga1–S6	2.243(3)
La1–S8×2	2.982(4)	La5–S7	3.092(3)	Ga1–S7	2.246(3)
La1–S7×2	2.984(3)	La5–S3	3.092(3)	Ga1–S8	2.260(3)
La1–S5×2	2.997(3)	La5–S1	3.092(3)	Ga1–S5	2.275(3)
La1–S4	3.024(4)	La5–S8	3.131(3)	Sb1–S3×2	2.454(3)
La2–S4	2.928(5)	La5–S5	3.135(3)	Sb1–S12	2.681(5)
La2–S5×2	2.970(3)	La5–S5	3.324(3)	Sb1–S4	2.747(4)
La2–S6×2	2.978(3)	La5–S8	3.327(3)	Sb2–S10×2	2.439(3)
La2–S8×2	3.003(3)	La5–S2	3.377(2)	Sb2–S11	2.539(4)
La2–S2	3.026(4)	Ba1–S10	3.203(3)	Sb2–S12	3.219(5)

La3–S9×2	2.902(3)	Ba1–S9×2	3.203(3)	Sb3–S9×2	2.435(3)
La3–S1×2	2.928(3)	Ba1–S10	3.221(3)	Sb3–S12	2.530(4)
La3–S6×2	3.011(3)	Ba1–S12	3.388(3)	Sb3–S11	3.216(5)
La3–S2	3.059(4)	Ba1–S11	3.389(2)	Sb4–S1×2	2.447(3)
La3–S11	3.098(5)	Ba1–S3	3.397(3)	Sb4–S11	2.675(5)
La4–S10×2	2.903(3)	Ba1–S1	3.401(3)	Sb4–S2	2.733(4)
La4–S3×2	2.935(3)	Ba1–S7	3.413(3)		
La4–S7×2	3.015(3)	Ba1–S6	3.421(3)		
La4–S4	3.069(5)				
La4–S12	3.098(4)				
La5–S6	3.091(3)				
La5–S7	3.092(3)				
La5–S3	3.092(3)				
La5–S1	3.092(3)				
La5–S8	3.131(3)				
La5–S5	3.135(3)				
La5–S5	3.324(3)				
La5–S8	3.327(3)				
La5–S2	3.377(2)				
La5–S4	3.379(2)				

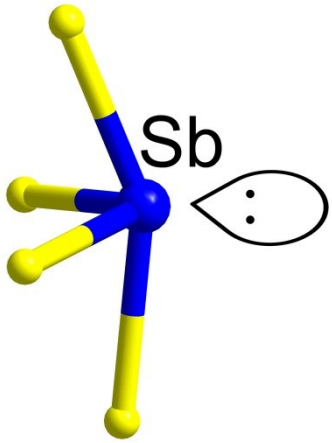


Figure S1. The teeter-totter polyhedron SbS_4. Legend: yellow, S; blue, Sb.

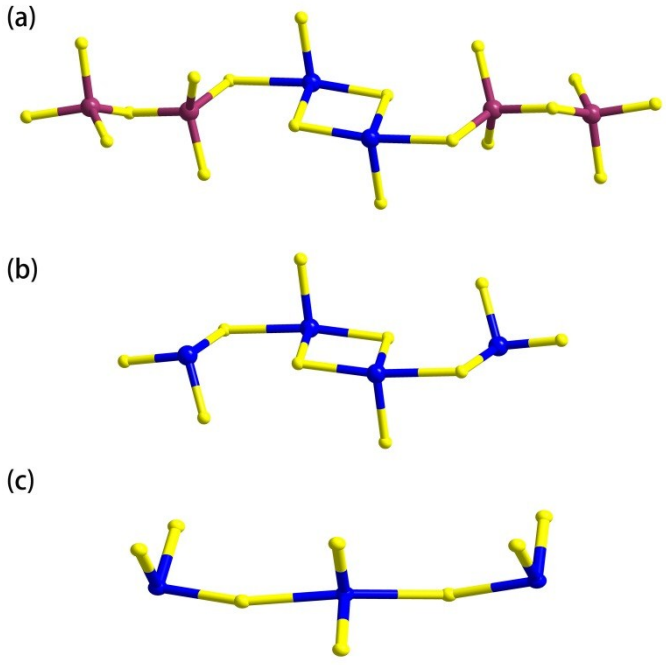
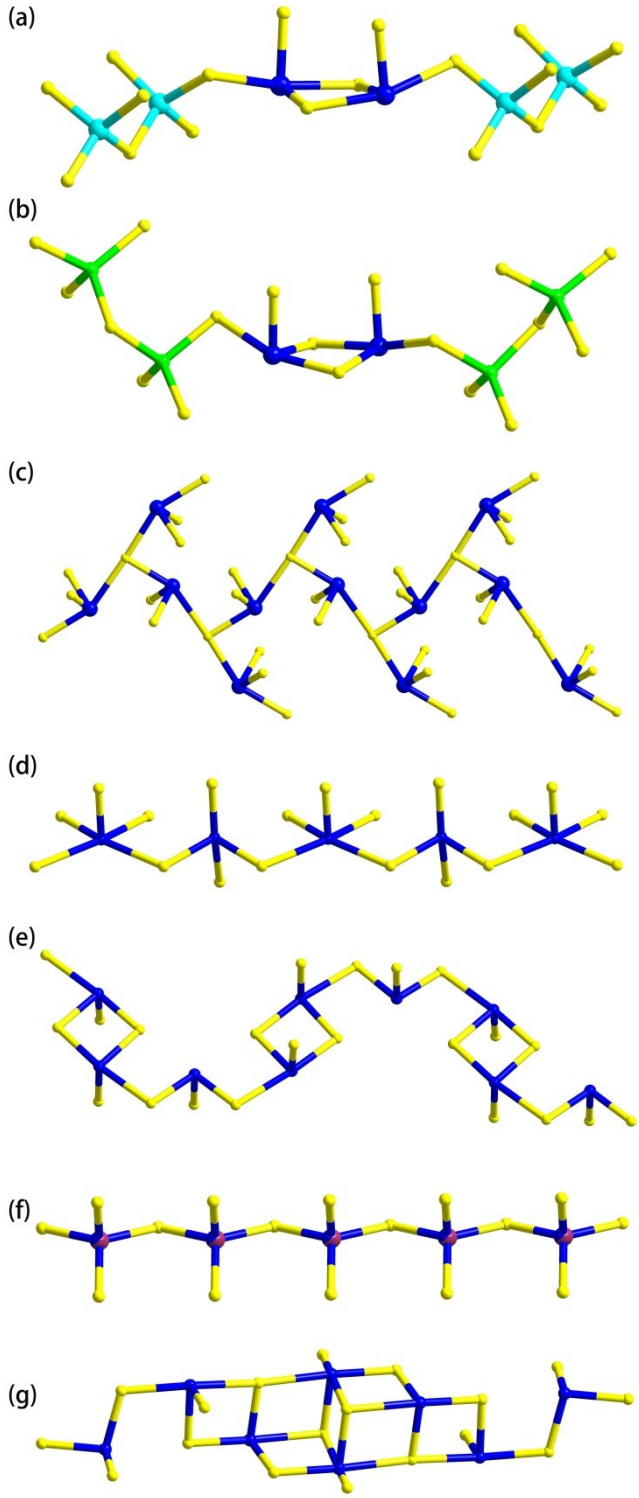


Figure S2. The isolated finite complex anion constructed by SbX_4 (X = S, Se) teeter-totter polyhedron connecting with other units in (a) $Ba_4LaGe_3SbSe_{13}$,[1] (b) $Ba_4Sb_3S_8Cl$,[2] and (c) $Ba_8Sb_6S_{17}$.[3] Legend: blue, Sb; dark red, Ge; yellow, S or Se.



Figrue S3. Infinite chains constructed by SbX_4 (X = S, Se) teeter-totter polyhedron connecting with other units in (a) Pr_4GaSbS_9,[4] (b) La_4InSbS_9,[5] (c) $La_4FeSb_2S_{10}$,[6] (d) $Ba_4SiSb_2Se_{11}$,[7] (e) $Na_9Gd_5Sb_8S_{26}$,[8] (f) $SrGeSb_2Se_8$,[9] and (g) $BaSb_2S_4$.[10] Legend: blue, Sb; light blue, Ga; green, In; blue and dark red, Ge/Sb; yellow, S or Se.

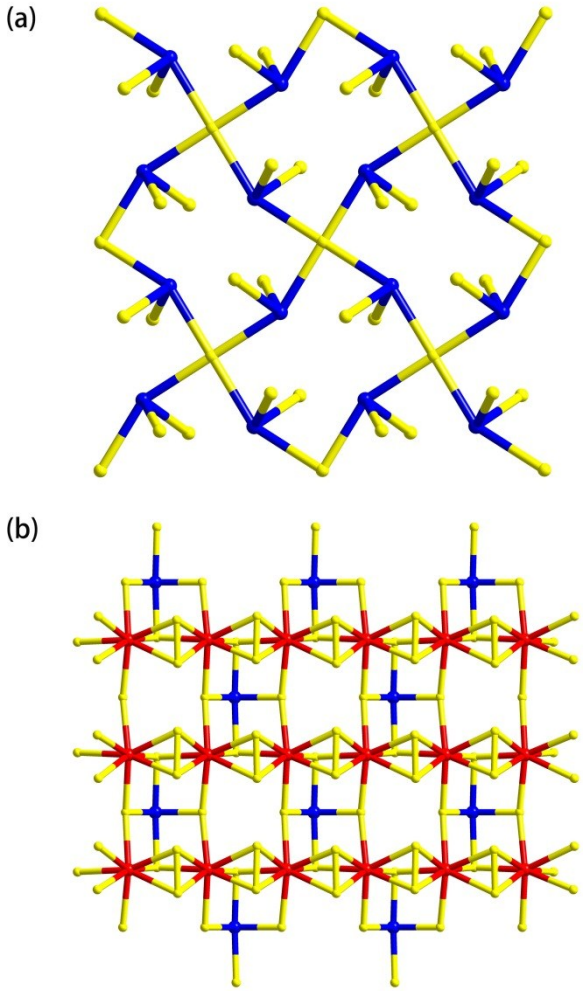


Figure S4. Layers constructed by SbS_4 teeter-totter polyhedron connecting with other units in $La_2Ga_{0.33}SbS_5$,[11] RbU_2SbS_8.[12] Legend: blue, Sb; red, U; yellow, S.

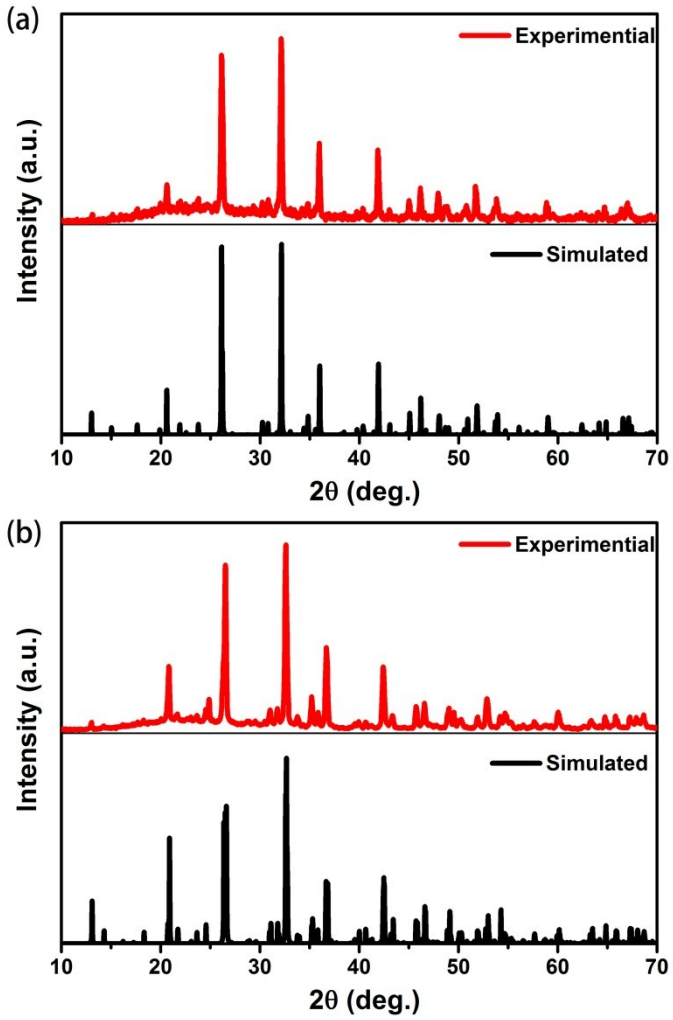


Figure S5. Experimental and simulated powder X-ray diffraction (XRD) data for (a) compound **1** and (b) **2**.

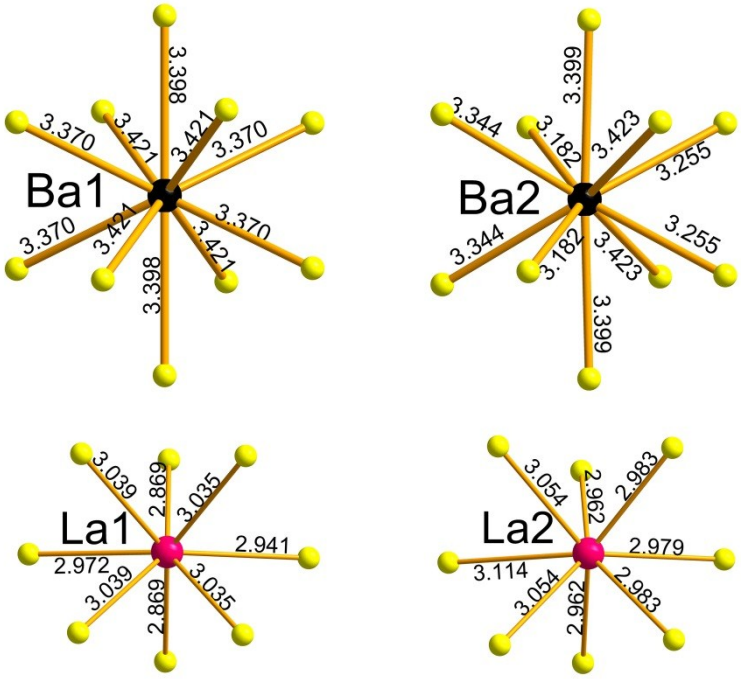


Figure S6. The coordination environment of Ba and La with S atoms in compound **1**

(The black, red and yellow balls represent Ba, La and S atoms, respectively)

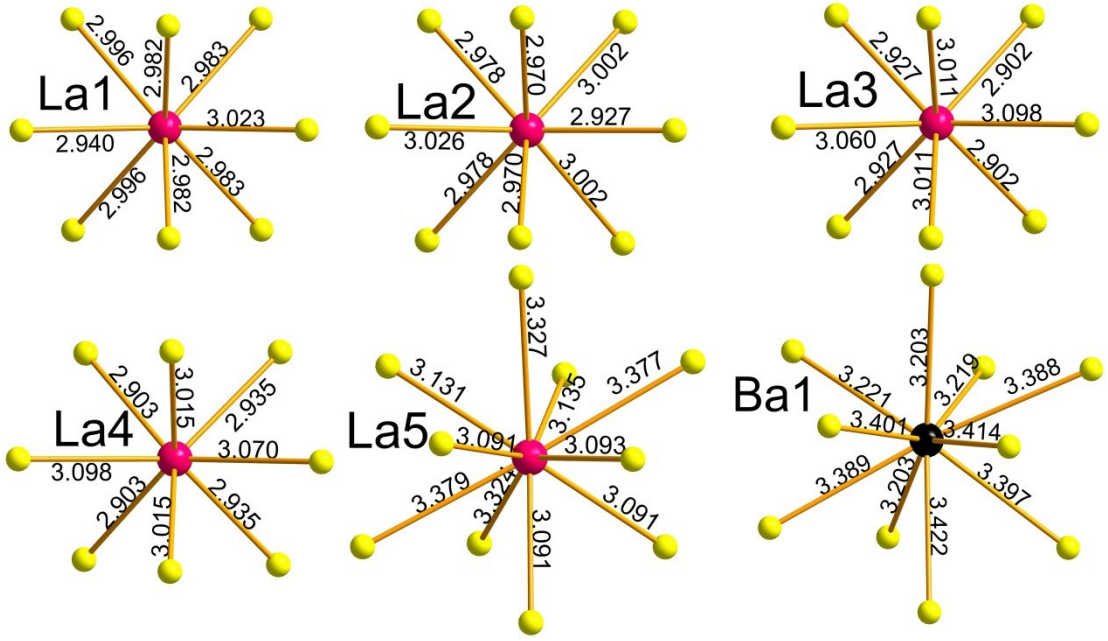


Figure S7. The coordination environment of La and Ba with S in compound **2** (The black, red and yellow balls represent Ba, La and S atoms, respectively)

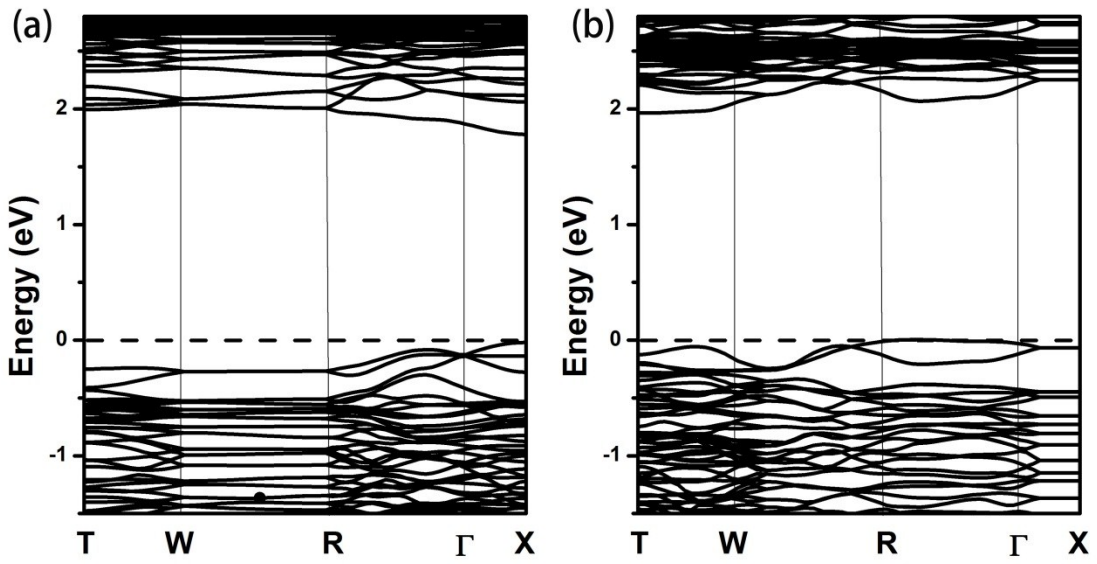


Figure S8. Calculated band structure of compound **1** (a) and **2** (b).

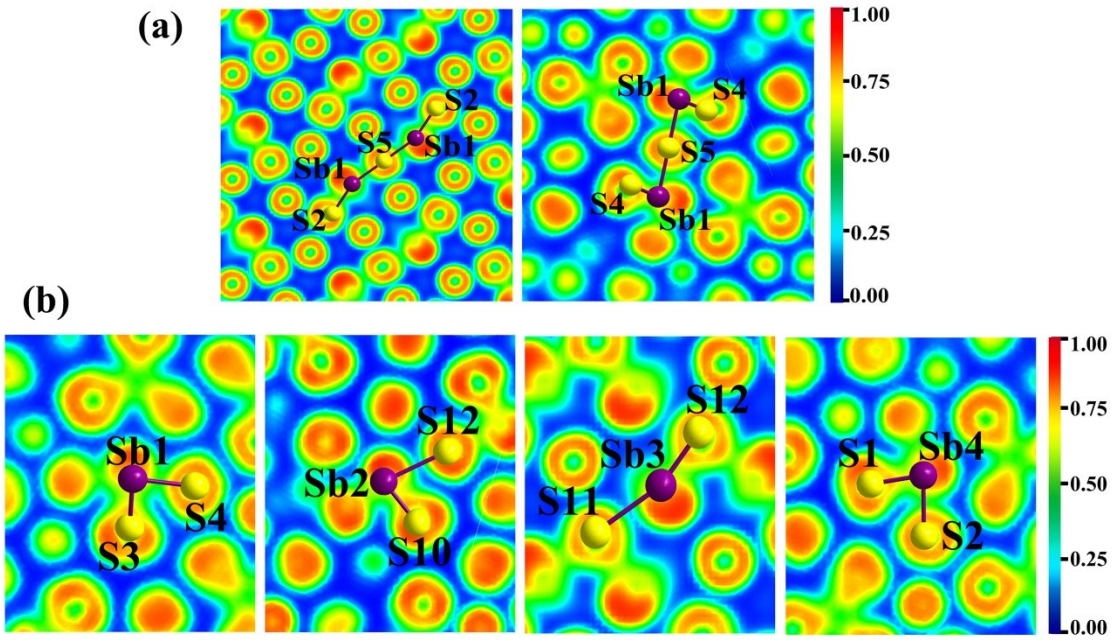


Figure S9. The Electron localization function (ELF) isofurfaces for the Sb–S bonds in compound **1** (a) and **2** (b). Contours are from 0.00 to 1.00.

Reference

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