

New quaternary chalcogenide $\text{Ba}_4\text{HgAs}_2\text{S}_{10}$ originating from the combination of linear $[\text{HgS}_2]^{2-}$ and tetrahedral $[\text{AsS}_4]^{3-}$ modules

Wenhao Xing,^{a, b, c, d} Naizheng Wang,^{a, c} Zhuang Li,^{a, c} Wenhao Liu,^a Jian Tang,^{b, d} Wenlong Yin,^{b, d*} Zheshuai Lin,^a Bin Kang,^{b, d} and Jiyong Yao^{a*}

^a Beijing Center for Crystal Research and Development, Key Lab of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China, corresponding author: Jiyong Yao, E-mail: jyao@mail.ipc.ac.cn.

^b Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, People's Republic of China. corresponding author: Wenlong Yin, E-mail: wlyin@caep.cn.

^c University of Chinese Academy of Sciences, Beijing 100049, P. R. China.

^d Key Laboratory of Science and Technology on High Energy Laser, China Academy of Engineering Physics, Mianyang 621900, People's Republic of China.

Table S1 Atomic coordinates, equivalent isotropic displacement parameters and bond valence sums (BVS) for Ba₄HgAs₂S₁₀.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}} (\text{\AA}^2)^a$	BVS
Hg1	0.5000	0.63849 (3)	0.7500	0.02033 (6)	1.980
Hg2	0.5000	1.0000	1.0000	0.02082 (7)	1.975
Ba1	0.68946 (2)	0.60340 (4)	0.70683 (2)	0.01969 (7)	1.864
Ba2	0.56505 (2)	1.10794 (3)	0.64831 (2)	0.01416 (6)	1.955
Ba3	0.56452 (2)	0.52898 (3)	0.89960 (2)	0.01489 (6)	1.936
Ba4	0.69072 (2)	1.00141 (3)	0.95371 (2)	0.01642 (7)	1.958
As1	0.64408 (2)	1.08286 (6)	0.79858 (2)	0.01109 (8)	5.005
As2	0.64423 (2)	0.52691 (5)	0.54873 (2)	0.01047 (8)	4.985
S1	0.55278 (4)	0.62475 (13)	0.67082 (3)	0.01428 (18)	2.035
S2	0.65655 (4)	0.77064 (14)	0.82631 (3)	0.0195 (2)	1.931
S3	0.55660 (4)	1.18888 (19)	0.78361 (4)	0.0285 (2)	1.806
S4	0.69083 (4)	1.29058 (15)	0.85035 (4)	0.0201 (2)	1.966
S5	6885.0(4)	10957.5(14)	7214.3(3)	14.45(19)	2.139
S6	5537.6(4)	10264.6(14)	9215.3(3)	14.54(18)	2.030
S7	6572.5(4)	8416.7(14)	5740.5(4)	20.1(2)	1.760
S8	5561.3(4)	4252.6(17)	5349.7(4)	21.9(2)	1.881
S9	6894.2(4)	3213.0(14)	6027.3(3)	16.45(18)	2.024
S10	6887.2(4)	4993.0(13)	4719.0(3)	13.63(19)	2.110

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

Table S2 Selected band distances (Å) and band angles (°) for Ba₄HgAs₂S₁₀.

Hg1—S1 ⁱ	2.3237(8)	Ba3—S4 ^{vi}	3.4920(10)
Hg1—S1	2.3237(8)	Ba3—S6	3.2751(9)
Hg2—S6 ⁱⁱⁱ	2.3246(8)	Ba3—S6 ^{vi}	3.3072(9)
Hg2—S6	2.3247(8)	Ba3—S8 ^x	3.4112(9)
Ba1—S1	3.2430(9)	Ba3—S8 ⁱ	3.2722(10)
Ba1—S2	3.2720(9)	Ba3—S10 ^x	3.3620(9)
Ba1—S4 ^{iv}	3.3121(10)	Ba4—S2	3.6085(10)
Ba1—S5 ^{iv}	3.3083(9)	Ba4—S4	3.1955(10)
Ba1—S5 ^{vi}	3.3055(10)	Ba4—S6	3.2252(9)
Ba1—S5	3.2071(10)	Ba4—S7 ⁱⁱ	3.2735(9)
Ba1—S9	3.1841(9)	Ba4—S9 ^v	3.2904(9)
Ba2—S1 ^{vii}	3.4032(9)	Ba4—S10 ^x	3.2724(9)
Ba2—S1	3.1897(9)	Ba4—S10 ⁱⁱ	3.2633(9)
Ba2—S3 ⁱ	3.2987(10)	Ba4—S10 ^v	3.3164(9)
Ba2—S3	3.4367(10)	As1—S2	2.1553(10)
Ba2—S5	3.3547(9)	As1—S3	2.1402(10)
Ba2—S6 ⁱ	3.2631(9)	As1—S4	2.1492(10)
Ba2—S7	3.2948(9)	As1—S5	2.1852(9)
Ba2—S8 ^{vii}	3.5104(10)	As2—S7	2.1538(10)
Ba2—S9 ^{vii}	3.3538(9)	As2—S8	2.1393(10)
Ba3—S1 ⁱ	3.2590(9)	As2—S9	2.1579(9)
Ba3—S2	3.1981(9)	As2—S10	2.1847(9)
Ba3—S3 ^{vi}	3.6503(12)		
S1 ⁱ —Hg1—S1	175.61(4)	S4—As1—S5	106.29(4)
S6 ⁱⁱⁱ —Hg2—S6	180.0	S7—As2—S9	109.45(4)
S2—As1—S5	105.08(4)	S7—As2—S10	105.85(4)
S3—As1—S2	118.63(5)	S8—As2—S7	117.84(4)
S3—As1—S4	111.44(5)	S8—As2—S9	110.97(4)
S3—As1—S5	105.38(4)	S8—As2—S10	105.62(4)
S4—As1—S2	109.07(4)	S9—As2—S10	106.30(4)

Symmetry codes: (i) $-x+1, y, -z+3/2$; (ii) $x, -y+2, z+1/2$; (iii) $-x+1, -y+2, -z+2$;
(iv) $-x+3/2, y-1/2, -z+3/2$; (v) $-x+3/2, y+1/2, -z+3/2$; (vi) $x, y-1, z$; (vii) $x, y+1, z$;
(viii) $-x+1, y+1, -z+3/2$; (ix) $-x+1, y-1, -z+3/2$; (x) $x, -y+1, z+1/2$; (xi) $-x+3/2, -y+5/2, -z+2$;
(xii) $x, -y+2, z-1/2$; (xiii) $x, -y+1, z-1/2$.

Synthesis of BaS₃

The binary material BaS₃ was synthesized by stoichiometric reaction of BaS and S element within a sealed silica tube. The tube was heated to 773 K in 10 h, maintained the temperature for 48 h, and then cooled down to room temperature by shutting off the furnace. In order to enhance the crystallinity and purity, the obtained sample was reground and the heat treatment was repeated. Eventually, yellow powder of BaS₃ was obtained. The measured powder X-ray diffraction (XRD) pattern agrees well with the simulated pattern from the reported single-crystal structure (ICSD #23637).

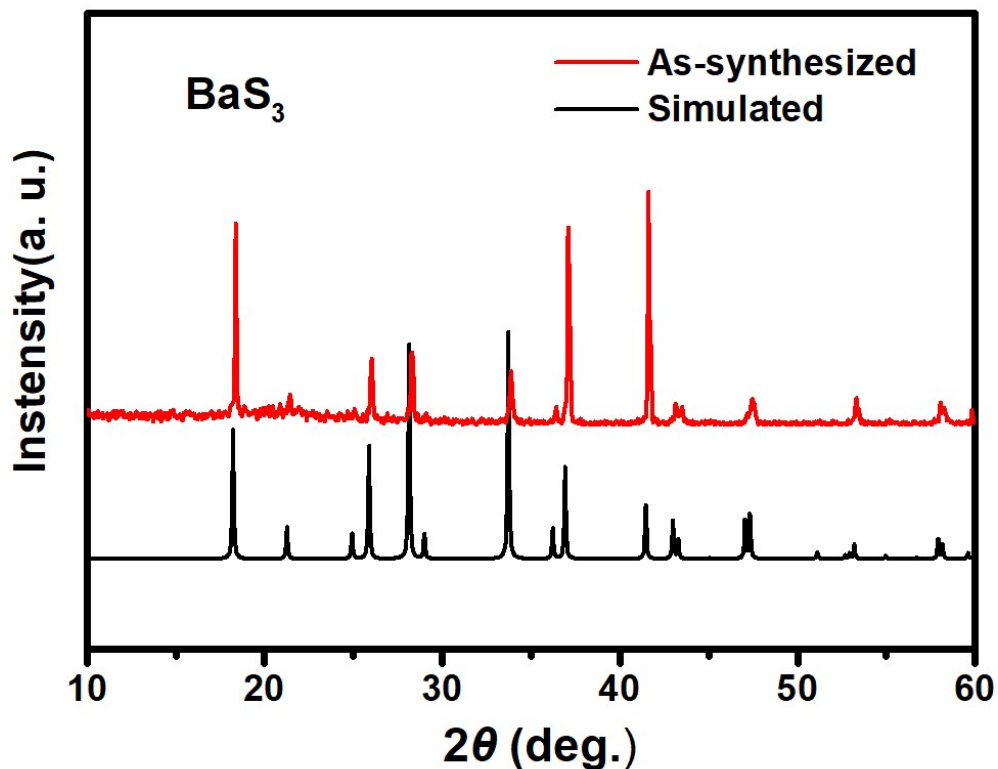


Figure S1. PXRD patterns of BaS₃.

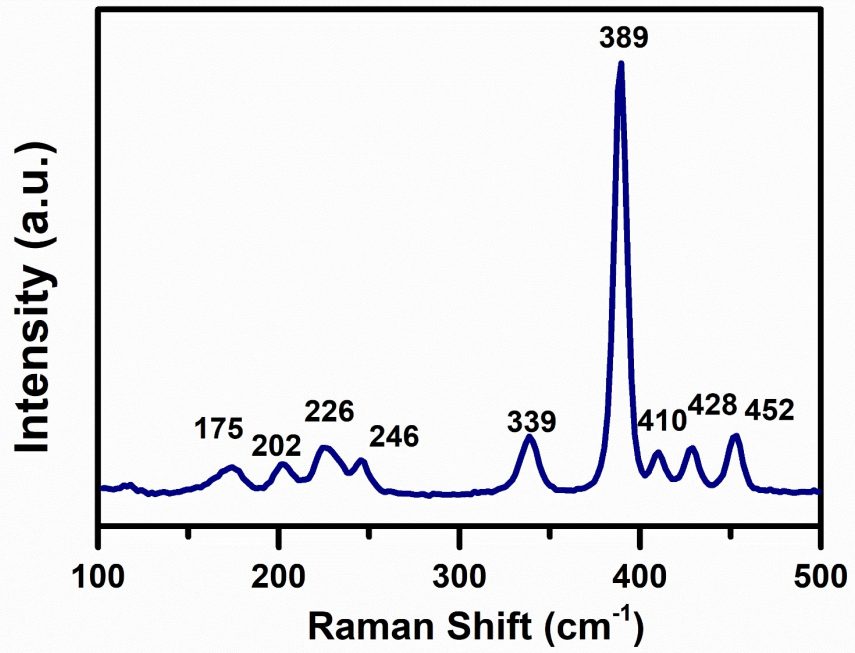


Figure S2. Raman spectrum of Ba₄HgAs₂S₁₀.

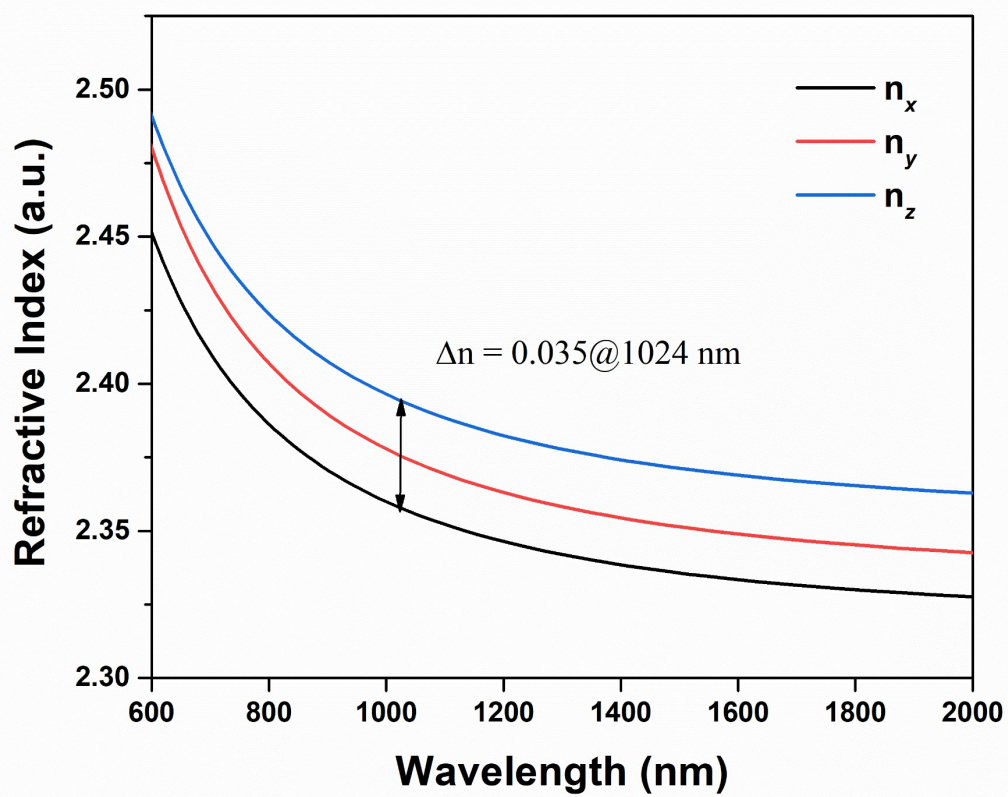


Figure S3. Refractive index dispersion diagrams of Ba₄HgAs₂S₁₀.