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Ba₂Sb₄GeS₁₀

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Sb}-\text{S}) = 0.001$ Å;
 R factor = 0.018; wR factor = 0.042; data-to-parameter ratio = 23.2.

The title quaternary compound, dibarium tetraantimony germanium decasulfide, Ba₂Sb₄GeS₁₀, crystallizes in a novel three-dimensional $\infty^3[\text{Sb}_4\text{GeS}_{10}]^{4-}$ network structure, which is composed of triangular pyramidal SbS₃ (site symmetry $m..$), distorted SbS₅ ($m..$) polyhedra and regular GeS₄ ($\bar{4}..$) tetrahedra. The SbS₃ and SbS₅ units are connected with each other through corner- and edge-sharing, forming a Sb₄S₁₀ layer in the ab plane. The GeS₄ tetrahedra further bridge two neighbouring Sb₄S₁₀ layers, forming a three-dimensional $\infty^3[\text{Sb}_4\text{GeS}_{10}]^{4-}$ network. The Ba²⁺ cation ($..2$) is located between two Sb₄S₁₀ layers and is coordinated by ten S atoms with Ba—S bond lengths in the range 3.2505 (9)–3.4121 (2) Å.

Related literature

The stereochemically active 5s² lone-pair electrons possess a large electric dipole moment and can influence structures that contain Sb³⁺, see: Choi & Kanatzidis (2000); Babo & Albrecht-Schmitt (2012). SbS₃, SbS₄ or SbS₅ units in a crystal structure are prone to form Sb—S chains through corner- or edge-sharing, see: Dorrscheidt & Schäfer (1981); Cordier *et al.* (1984). GeS₄ tetrahedra can be utilized as the second structural unit and introduced into crystal structures to connect Sb—S chains into a two-dimensional layer or three-dimensional framework structure (Feng *et al.*, 2008). For crystal structures and optical properties, see: Deng *et al.* (2005); Kim *et al.* (2008); Ribes *et al.* (1973); Teske (1979); Lekse *et al.* (2009).

Experimental

Crystal data

Ba₂Sb₄GeS₁₀ $M_r = 1154.87$

Tetragonal, $P4_2/mbc$
 $a = 11.3119$ (4) Å
 $c = 13.6384$ (9) Å
 $V = 1745.16$ (14) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 13.40$ mm⁻¹
 $T = 293$ K
 $0.22 \times 0.07 \times 0.07$ mm

Data collection

Rigaku SCXMini CCD
diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2007)
 $T_{\min} = 0.530$, $T_{\max} = 1.000$

12411 measured reflections
1046 independent reflections
1032 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.018$
 $wR(F^2) = 0.042$
 $S = 1.15$
1046 reflections

45 parameters
 $\Delta\rho_{\max} = 0.66$ e Å⁻³
 $\Delta\rho_{\min} = -0.74$ e Å⁻³

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2163).

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supporting information

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Ba₂Sb₄GeS₁₀**Lei Geng****S1. Comment**

Sb-based chalcogenides have attracted a lot of attention in recent years due to their rich structures and interesting physical properties, such as nonlinear optics and ion-exchange properties. The stereochemically active 5 s² lone-pair electrons possess a large electric dipole moment and can influence structures that contain Sb³⁺ (Choi *et al.* 2000; Babo *et al.* 2012). SbS₃, SbS₄ or SbS₅ units in a crystal structure are prone to form one-dimensional Sb—S chains through a corner- or edge-sharing manner (Dorrscheidt *et al.* 1981; Cordier *et al.* 1984). GeS₄ tetrahedron can be utilized as the second structural unit and introduced into crystal structure to connect Sb—S chains into a two-dimensional layer or three-dimensional framework structure (Feng *et al.* 2008). In this paper, a new title quaternary sulfide in the Sb—Ge—S system is described. Ba₂Sb₄GeS₁₀ represents the first example of a structure synthesized and structurally characterized by single-crystal X-ray diffraction in the quaternary Ba—Sb—Ge—S system (Fig. 1). It crystallizes with one Ge atom on 4*b* and three S atoms on 8*h*, 16*i* and 16*i*, respectively, in terms of the Wyckoff notation. There are two types of coordination polyhedron of SbS groups, *i.e.* triangle-pyramidal SbS₃ and distorted SbS₅ polyhedra. SbS₃ and SbS₅ polyhedra are connected with each other through corner- and edge-sharing conformations to form Sb₄S₁₀ zigzag chains, which are further arranged side by side into the Sb₄S₁₀ layer in the *ab*-plane (Fig. 2). The GeS₄ tetrahedra further bridge two neighbouring Sb₄S₁₀ layers, forming a three-dimensional ∞³[Sb₄GeS₁₀]⁴⁻ network (Fig. 3). The Ba atom is located between two Sb₄S₁₀ layers and coordinates with ten S atoms with Ba—S bonding lengths in the range of 3.2505 (9)–3.4121 (2) Å, which are typical values for sulfides (Dorrscheidt *et al.* 1981; Cordier *et al.* 1984).

S2. Experimental

The title compound, Ba₂Sb₄GeS₁₀, was synthesized through a high temperature solid-state reaction in an evacuated and sealed silica tube. A mixture of BaS (0.5 mmol, 0.0847 g), Sb (1 mmol, 0.1218 g), Ge (0.25 mmol, 0.0182 g), S (2 mmol, 0.0641 g) was loaded in a silica ampoule, sealed under 10⁻² Pa, heated gradually to 1173 K (holding for 10 h) in 60 h, and then cooled to room temperature in 300 h. Rod-shaped crystals of Ba₂Sb₄GeS₁₀ with a dark red color were obtained. The crystals were stable under air and moisture conditions.

S3. Refinement

All atoms in Ba₂Sb₄GeS₁₀ crystal structure were refined anisotropically without disorder. The highest residual peak (0.66 e⁻Å⁻³) in the difference electron density map was located at (0.1992, 0.3008, 1/4), 1.09 Å from atom Ba1. The deepest hole (-0.73 e⁻Å⁻³) was located at (0.1670, 0.7496, 0.2499), 0.77 Å from atom Ba1.

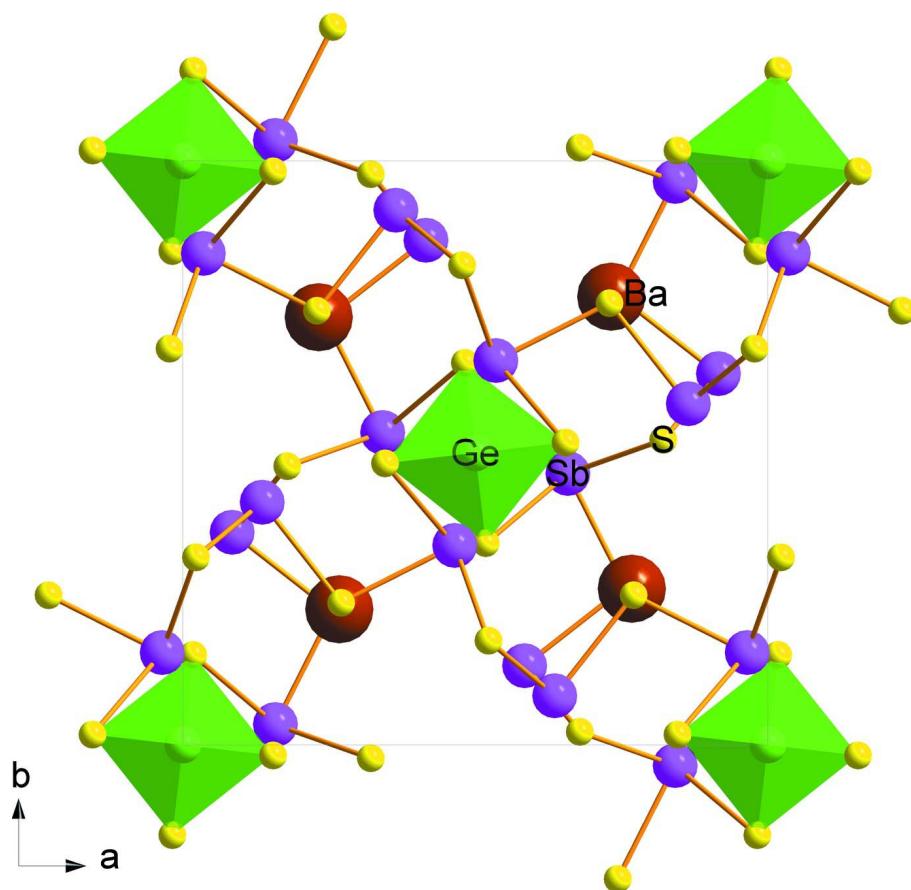


Figure 1

Crystal structure of Ba₂Sb₄GeS₁₀ in GeS₄ polyhedral representation viewed along [001]. Green tetrahedra represent the GeS₄ unit with yellow sulfur atoms at the corners of each tetrahedron.

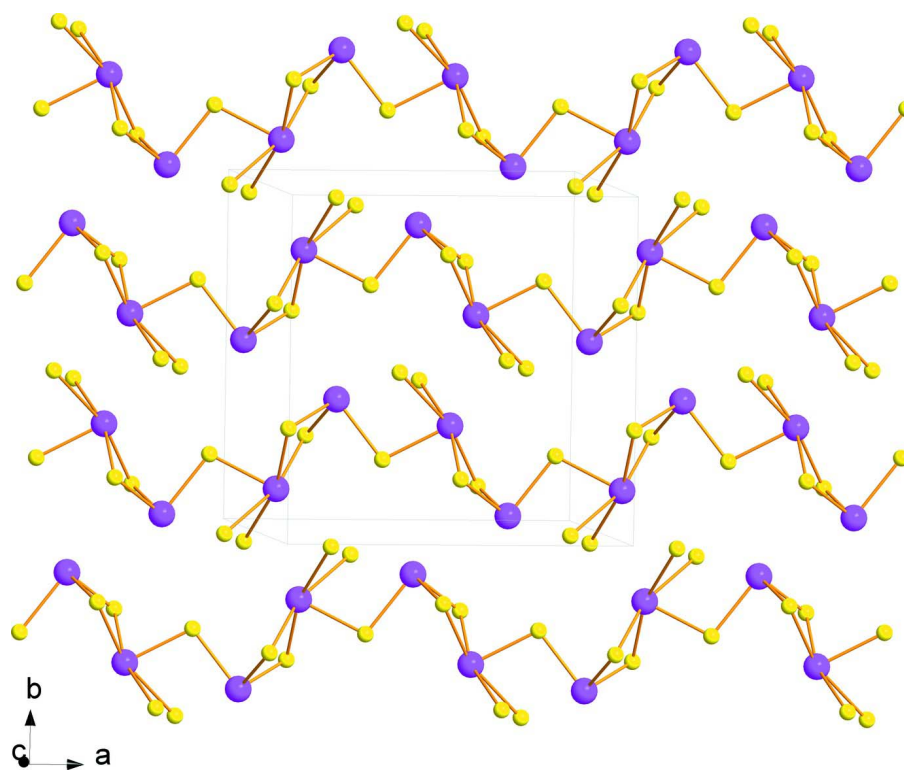


Figure 2

SbS_3 and SbS_5 polyhedra are connected with each other through corner- and edge-sharing conformations to form the Sb_4S_{10} zigzag chains, which are further arranged side by side into the Sb_4S_{10} layer in the ab -plane.

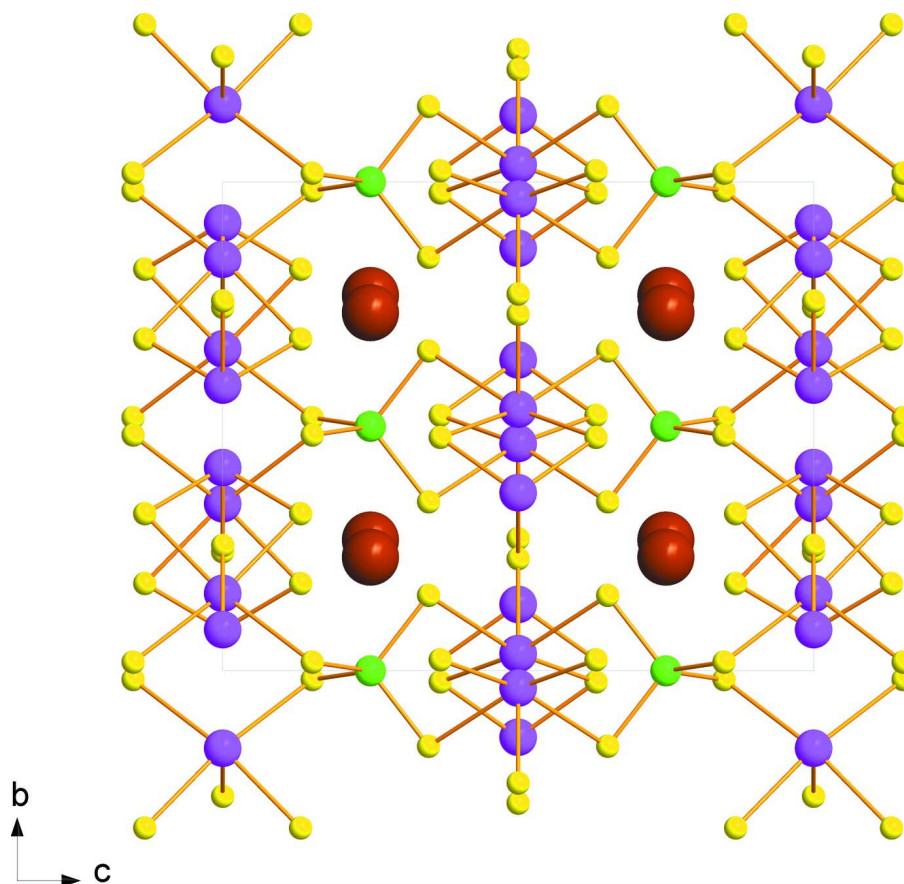


Figure 3

The novel three-dimensional $\infty^3[\text{Sb}_4\text{GeS}_{10}]^{-4}$ network viewed along $[100]$ direction. GeS_4 tetrahedra act as bridging units for two neighbouring Sb_4S_{10} layers.

Dibarium tetraantimony(III) germanium(IV) decasulfide

Crystal data

$\text{Ba}_2\text{Sb}_4\text{GeS}_{10}$

$M_r = 1154.87$

Tetragonal, $P4_2/mbc$

Hall symbol: $-P\ 4ac\ 2ab$

$a = 11.3119\ (4)\ \text{\AA}$

$c = 13.6384\ (9)\ \text{\AA}$

$V = 1745.16\ (14)\ \text{\AA}^3$

$Z = 4$

$F(000) = 2032$

$D_x = 4.395\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1877 reflections

$\theta = 2.3\text{--}27.5^\circ$

$\mu = 13.40\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Rod, dark-red

$0.22 \times 0.07 \times 0.07\ \text{mm}$

Data collection

Rigaku SCXMini CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

CCD_Profile_fitting scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2007)

$T_{\min} = 0.530$, $T_{\max} = 1.000$

12411 measured reflections

1046 independent reflections

1032 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -14 \rightarrow 14$

$k = -14 \rightarrow 11$

$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0214P)^2 + 3.2912P]$
$R[F^2 > 2\sigma(F^2)] = 0.018$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.042$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.15$	$\Delta\rho_{\max} = 0.66 \text{ e } \text{\AA}^{-3}$
1046 reflections	$\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$
45 parameters	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.00225 (8)
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba1	0.232424 (19)	0.732424 (19)	0.2500	0.01704 (10)
Sb1	0.13578 (3)	0.41567 (3)	0.0000	0.01543 (10)
Sb2	0.46488 (3)	0.34169 (3)	0.0000	0.01796 (10)
Ge1	0.0000	0.0000	0.2500	0.01175 (15)
S1	0.27060 (10)	0.24355 (10)	0.0000	0.0136 (2)
S2	0.01781 (8)	0.15428 (7)	0.34843 (6)	0.01631 (18)
S3	0.02261 (7)	0.32137 (8)	0.13186 (6)	0.01777 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01715 (12)	0.01715 (12)	0.01683 (15)	0.00214 (11)	-0.00097 (7)	0.00097 (7)
Sb1	0.01518 (17)	0.01341 (17)	0.01771 (17)	0.00143 (11)	0.000	0.000
Sb2	0.01151 (17)	0.02030 (18)	0.02206 (18)	-0.00225 (12)	0.000	0.000
Ge1	0.0126 (2)	0.0126 (2)	0.0101 (3)	0.000	0.000	0.000
S1	0.0101 (5)	0.0121 (5)	0.0184 (6)	-0.0006 (4)	0.000	0.000
S2	0.0201 (4)	0.0142 (4)	0.0146 (4)	-0.0020 (3)	-0.0009 (3)	-0.0026 (3)
S3	0.0131 (4)	0.0254 (4)	0.0147 (4)	-0.0025 (3)	0.0024 (3)	-0.0028 (3)

Geometric parameters (\AA , $^\circ$)

Ba1—S2 ⁱ	3.2505 (9)	Sb2—S3 ^{viii}	2.6576 (9)
Ba1—S2 ⁱⁱ	3.2505 (9)	Sb2—S2 ^{iv}	2.9352 (9)
Ba1—S3 ⁱⁱ	3.3596 (9)	Sb2—S2 ^{ix}	2.9352 (9)
Ba1—S3 ⁱ	3.3596 (9)	Ge1—S2	2.2110 (8)

Ba1—S3 ⁱⁱⁱ	3.3599 (8)	Ge1—S2 ^x	2.2110 (8)
Ba1—S3 ^{iv}	3.3599 (8)	Ge1—S2 ^{xi}	2.2110 (8)
Ba1—S2 ^{iv}	3.3849 (9)	Ge1—S2 ^{xii}	2.2110 (8)
Ba1—S2 ⁱⁱⁱ	3.3849 (9)	S1—Ba1 ^{xiii}	3.4121 (2)
Ba1—S1 ⁱⁱ	3.4121 (2)	S1—Ba1 ^{xiv}	3.4121 (2)
Ba1—S1 ^v	3.4121 (2)	S2—Sb2 ^{xv}	2.9352 (9)
Sb1—S3 ^{vi}	2.4517 (9)	S2—Ba1 ^{xiv}	3.2505 (9)
Sb1—S3	2.4517 (9)	S2—Ba1 ⁱⁱⁱ	3.3849 (9)
Sb1—S1	2.4732 (12)	S3—Sb2 ^{xvi}	2.6576 (9)
Sb2—S1	2.4621 (12)	S3—Ba1 ^{xiv}	3.3596 (9)
Sb2—S3 ^{vii}	2.6576 (9)	S3—Ba1 ⁱⁱⁱ	3.3599 (8)
S2 ⁱ —Ba1—S2 ⁱⁱ	130.04 (3)	S3 ^{iv} —Ba1—S1 ^v	120.60 (3)
S2 ⁱ —Ba1—S3 ⁱⁱ	76.46 (2)	S2 ^{iv} —Ba1—S1 ^v	68.80 (2)
S2 ⁱⁱ —Ba1—S3 ⁱⁱ	64.06 (2)	S2 ⁱⁱⁱ —Ba1—S1 ^v	111.96 (2)
S2 ⁱ —Ba1—S3 ⁱ	64.06 (2)	S1 ⁱⁱ —Ba1—S1 ^v	177.82 (4)
S2 ⁱⁱ —Ba1—S3 ⁱ	76.46 (2)	S3 ^{vi} —Sb1—S3	94.37 (4)
S3 ⁱⁱ —Ba1—S3 ⁱ	74.69 (3)	S3 ^{vi} —Sb1—S1	88.82 (3)
S2 ⁱ —Ba1—S3 ⁱⁱⁱ	153.52 (2)	S3—Sb1—S1	88.82 (3)
S2 ⁱⁱ —Ba1—S3 ⁱⁱⁱ	74.09 (2)	S1—Sb2—S3 ^{vii}	84.63 (3)
S3 ⁱⁱ —Ba1—S3 ⁱⁱⁱ	129.53 (3)	S1—Sb2—S3 ^{viii}	84.63 (3)
S3 ⁱ —Ba1—S3 ⁱⁱⁱ	122.17 (3)	S3 ^{vii} —Sb2—S3 ^{viii}	85.17 (4)
S2 ⁱ —Ba1—S3 ^{iv}	74.09 (2)	S1—Sb2—S2 ^{iv}	80.46 (3)
S2 ⁱⁱ —Ba1—S3 ^{iv}	153.52 (2)	S3 ^{vii} —Sb2—S2 ^{iv}	164.84 (3)
S3 ⁱⁱ —Ba1—S3 ^{iv}	122.17 (3)	S3 ^{viii} —Sb2—S2 ^{iv}	90.69 (3)
S3 ⁱ —Ba1—S3 ^{iv}	129.53 (3)	S1—Sb2—S2 ^{ix}	80.46 (3)
S3 ⁱⁱⁱ —Ba1—S3 ^{iv}	85.35 (3)	S3 ^{vii} —Sb2—S2 ^{ix}	90.69 (3)
S2 ⁱ —Ba1—S2 ^{iv}	66.88 (3)	S3 ^{viii} —Sb2—S2 ^{ix}	164.84 (3)
S2 ⁱⁱ —Ba1—S2 ^{iv}	131.76 (3)	S2 ^{iv} —Sb2—S2 ^{ix}	89.54 (3)
S3 ⁱⁱ —Ba1—S2 ^{iv}	140.05 (2)	S2—Ge1—S2 ^x	111.63 (2)
S3 ⁱ —Ba1—S2 ^{iv}	75.40 (2)	S2—Ge1—S2 ^{xi}	105.23 (4)
S3 ⁱⁱⁱ —Ba1—S2 ^{iv}	89.05 (2)	S2 ^x —Ge1—S2 ^{xi}	111.63 (2)
S3 ^{iv} —Ba1—S2 ^{iv}	62.66 (2)	S2—Ge1—S2 ^{xii}	111.63 (2)
S2 ⁱ —Ba1—S2 ⁱⁱⁱ	131.76 (3)	S2 ^x —Ge1—S2 ^{xii}	105.23 (4)
S2 ⁱⁱ —Ba1—S2 ⁱⁱⁱ	66.88 (3)	S2 ^{xi} —Ge1—S2 ^{xii}	111.63 (2)
S3 ⁱⁱ —Ba1—S2 ⁱⁱⁱ	75.40 (2)	Sb2—S1—Sb1	101.27 (4)
S3 ⁱ —Ba1—S2 ⁱⁱⁱ	140.05 (2)	Sb2—S1—Ba1 ^{xiii}	91.466 (19)
S3 ⁱⁱⁱ —Ba1—S2 ⁱⁱⁱ	62.66 (2)	Sb1—S1—Ba1 ^{xiii}	91.31 (2)
S3 ^{iv} —Ba1—S2 ⁱⁱⁱ	89.05 (2)	Sb2—S1—Ba1 ^{xiv}	91.466 (19)
S2 ^{iv} —Ba1—S2 ⁱⁱⁱ	142.24 (3)	Sb1—S1—Ba1 ^{xiv}	91.31 (2)
S2 ⁱ —Ba1—S1 ⁱⁱ	63.42 (2)	Ba1 ^{xiii} —S1—Ba1 ^{xiv}	175.62 (4)
S2 ⁱⁱ —Ba1—S1 ⁱⁱ	115.56 (2)	Ge1—S2—Sb2 ^{xv}	96.58 (3)
S3 ⁱⁱ —Ba1—S1 ⁱⁱ	61.18 (2)	Ge1—S2—Ba1 ^{xiv}	92.47 (3)
S3 ⁱ —Ba1—S1 ⁱⁱ	116.86 (3)	Sb2 ^{xv} —S2—Ba1 ^{xiv}	86.85 (2)
S3 ⁱⁱⁱ —Ba1—S1 ⁱⁱ	120.60 (3)	Ge1—S2—Ba1 ⁱⁱⁱ	88.96 (3)
S3 ^{iv} —Ba1—S1 ⁱⁱ	61.24 (2)	Sb2 ^{xv} —S2—Ba1 ⁱⁱⁱ	154.96 (3)
S2 ^{iv} —Ba1—S1 ⁱⁱ	111.96 (2)	Ba1 ^{xiv} —S2—Ba1 ⁱⁱⁱ	117.39 (2)
S2 ⁱⁱⁱ —Ba1—S1 ⁱⁱ	68.80 (2)	Sb1—S3—Sb2 ^{xvi}	86.21 (3)

S2 ⁱ —Ba1—S1 ^v	115.56 (2)	Sb1—S3—Ba1 ^{xiv}	92.95 (3)
S2 ⁱⁱ —Ba1—S1 ^v	63.42 (2)	Sb2 ^{xvi} —S3—Ba1 ^{xiv}	108.63 (3)
S3 ⁱⁱ —Ba1—S1 ^v	116.86 (3)	Sb1—S3—Ba1 ⁱⁱⁱ	151.51 (4)
S3 ⁱ —Ba1—S1 ^v	61.18 (2)	Sb2 ^{xvi} —S3—Ba1 ⁱⁱⁱ	89.30 (2)
S3 ⁱⁱⁱ —Ba1—S1 ^v	61.24 (2)	Ba1 ^{xiv} —S3—Ba1 ⁱⁱⁱ	115.09 (3)
S3 ^{vii} —Sb2—S1—Sb1	-137.18 (2)	S3—Sb1—S1—Ba1 ^{xiv}	-41.05 (3)
S3 ^{viii} —Sb2—S1—Sb1	137.18 (2)	S2 ^x —Ge1—S2—Sb2 ^{xv}	157.74 (2)
S2 ^{iv} —Sb2—S1—Sb1	45.572 (18)	S2 ^{xi} —Ge1—S2—Sb2 ^{xv}	36.474 (13)
S2 ^{ix} —Sb2—S1—Sb1	-45.572 (18)	S2 ^{xii} —Ge1—S2—Sb2 ^{xv}	-84.791 (7)
S3 ^{vii} —Sb2—S1—Ba1 ^{xiii}	-45.55 (3)	S2 ^x —Ge1—S2—Ba1 ^{xiv}	-115.15 (4)
S3 ^{viii} —Sb2—S1—Ba1 ^{xiii}	-131.19 (3)	S2 ^{xi} —Ge1—S2—Ba1 ^{xiv}	123.59 (3)
S2 ^{iv} —Sb2—S1—Ba1 ^{xiii}	137.20 (3)	S2 ^{xii} —Ge1—S2—Ba1 ^{xiv}	2.32 (3)
S2 ^{ix} —Sb2—S1—Ba1 ^{xiii}	46.06 (2)	S2 ^x —Ge1—S2—Ba1 ⁱⁱⁱ	2.23 (2)
S3 ^{vii} —Sb2—S1—Ba1 ^{xiv}	131.19 (3)	S2 ^{xi} —Ge1—S2—Ba1 ⁱⁱⁱ	-119.04 (3)
S3 ^{viii} —Sb2—S1—Ba1 ^{xiv}	45.55 (3)	S2 ^{xii} —Ge1—S2—Ba1 ⁱⁱⁱ	119.70 (3)
S2 ^{iv} —Sb2—S1—Ba1 ^{xiv}	-46.06 (2)	S3 ^{vi} —Sb1—S3—Sb2 ^{xvi}	22.13 (4)
S2 ^{ix} —Sb2—S1—Ba1 ^{xiv}	-137.20 (3)	S1—Sb1—S3—Sb2 ^{xvi}	-66.60 (3)
S3 ^{vi} —Sb1—S1—Sb2	132.80 (2)	S3 ^{vi} —Sb1—S3—Ba1 ^{xiv}	130.615 (18)
S3—Sb1—S1—Sb2	-132.80 (2)	S1—Sb1—S3—Ba1 ^{xiv}	41.89 (3)
S3 ^{vi} —Sb1—S1—Ba1 ^{xiii}	41.05 (3)	S3 ^{vi} —Sb1—S3—Ba1 ⁱⁱⁱ	-59.38 (9)
S3—Sb1—S1—Ba1 ^{xiii}	135.44 (3)	S1—Sb1—S3—Ba1 ⁱⁱⁱ	-148.11 (7)
S3 ^{vi} —Sb1—S1—Ba1 ^{xiv}	-135.44 (3)		

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