Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# Schaurteite, $Ca_3Ge(SO_4)_2(OH)_6{\cdot}3H_2O$

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Received 27 November 2012; accepted 14 December 2012

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(S–O) = 0.002 Å; $R$ factor = 0.022; $wR$ factor = 0.045; data-to-parameter ratio = 15.3.

This report presents the first crystal structure determination of the mineral schaurteite, ideally $Ca_3Ge(SO_4)_2(OH)_6{\cdot}3H_2O$, tricalcium germanium bis(sulfate) hexahydroxide trihydrate. This single-crystal X-ray diffraction study investigated a natural sample from the type locality at Tsumeb, Namibia. Schaurteite is a member of the fleischerite group of minerals, which also includes fleischerite, despujolsite, and mallestigite. The structure of schaurteite consists of slabs of $Ca(O,OH,H_2O)_8$ polyhedra (site symmetry $mm2$) interleaved with a mixed layer of $Ge(OH)_6$ octahedra ($\overline{3}m.$) and $SO_4$ tetrahedra ($3m.$). There are two H atoms in the asymmetric unit, both located by full-matrix refinement, and both forming O—H$\cdots$O hydrogen bonds.

## Related literature

For the original description of schaurteite, see: Strunz & Tennyson (1967). For descriptions of related minerals: fleischerite (Frondel & Strunz, 1960); despujolsite (Gaudefroy *et al.*, 1968); mallestigite (Sima *et al.*, 1996). For structural refinements of related minerals: despujolsite (Barkley *et al.*, 2011); fleischerite (Otto, 1975). For analysis of anisotropic displacement parameters, see: Downs (2000).

## Experimental

### *Crystal data*

$Ca_3Ge(SO_4)_2(OH)_6(H_2O)_3$
$M_r$ = 541.05
Hexagonal, $P6_3/mmc$
$a$ = 8.5253 (4) Å
$c$ = 10.8039 (6) Å
$V$ = 680.03 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 3.79 mm$^{-1}$
$T$ = 296 K
0.05 × 0.03 × 0.03 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
$T_{\min}$ = 0.656, $T_{\max}$ = 0.747
17243 measured reflections
536 independent reflections
456 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.061

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.045
$S$ = 1.15
536 reflections
35 parameters
All H-atom parameters refined
$\Delta\rho_{\max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.42 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O3—H1$\cdots$O2$^{\rm i}$ | 0.73 (3) | 2.12 (3) | 2.823 (2) | 164 (3) |
| O4—H2$\cdots$O1$^{\rm ii}$ | 0.79 (3) | 2.04 (3) | 2.789 (2) | 158 (3) |

Symmetry codes: (i) $y, x, -z$; (ii) $y, -x+y, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XtalDraw* (Downs & Hall-Wallace, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank the Arizona Science Foundation for their support. Thanks to Stephen G. West for systems support. This paper benefited greatly from the comments of Sean Parkin, who recognized the likehood of centrosymmetry in schaurteite.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2217).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, i6 [doi:10.1107/S1600536812050945]

## Schaurteite, $Ca_3Ge(SO_4)_2(OH)_6{\cdot}3H_2O$

**Marcus J. Origlieri and Robert T. Downs**

### Comment

Schaurteite, $Ca_3Ge(SO_4)_2(OH)_6.3H_2O$, is a rare germanium mineral found in oxidized germanite ores at the Tsumeb Corporation mine, Tsumeb, Namibia (Strunz & Tennyson, 1967). Schaurteite belongs to the fleischerite group of isotypic minerals, along with mallestigite, $Pb_3Sb(SO_4)(AsO_4)(OH)_6.3H_2O$ (Sima *et al.* 1996), despujolsite, $Ca_3Mn^{4+}(SO_4)_2(OH)_6.3H_2O$ (Gaudefroy *et al.* 1968), and fleischerite, $Pb_3Ge(SO_4)_2(OH)_6.3H_2O$ (Frondel & Strunz, 1960). Of these four minerals, only despujolsite (Barkley *et al.* 2011) and synthetic fleischerite (Otto, 1975) have reported structures. This study represents the first structural report for schaurteite.

The crystal structure of schaurteite consists of slabs of $Ca(OH)_4O_2(H_2O)_2$ polyhedra (*mm.* symmetry), interconnected by mixed layers of $Ge(OH)_6$ octahedra ($\bar{3}m.$ symmetry) and $SO_4$ tetrahedra ($3m.$ symmetry) (Figures 1,2). The mean Ca—O, Ge—O, and S—O bond lengths are 2.487 Å, 1.895 Å, and 1.468 Å, respectively. There are two separate hydrogen atoms, H1 bonded to the O3 atom coordinating Ge, and H2 bonded to the O4 atom (*mm.* symmetry) which generates an $H_2O$ molecule. Both H atoms form hydrogen bonds, O3—H1···O2 and O4—H2···O1 (Figure 3), mimicking those seen in despujolsite (Barkley *et al.* 2011).

In the original description of schaurteite, Strunz and Tennyson (1967) noted systematic absences in X-ray photographs consistent with three different space groups: $P6_3/mmc$, $P6_3mc$, and $P\bar{6}2c$. Supposing an isostructural relationship with despujolsite (Barkley *et al.* 2011), this study initially refined schaurteite in space group $P\bar{6}2c$ with a favorable $R_{obs}$ of 0.0251 for 45 parameters. Despite the relatively low $R$ factor, the positional parameters for H2 did not converge, and a twin model showed a racemic component of 47%, indicating centrosymmetry in the structure. In space group $P6_3/mmc$, the structural refinement converged rapidly for all atomic coordinates including those for H, and $R_{obs}$ dropped to .0219 for 35 parameters. Consequently, this study proposes $P6_3/mmc$ symmetry for schaurteite, in contrast to $P\bar{6}2c$ symmetry reported for both fleischerite (Otto, 1975) and despujolsite (Barkley *et al.* 2011). Curiously, schaurteite, $Ca_3Ge(SO_4)_2(OH)_6.3H_2O$, and fleischerite, $Pb_3Ge(SO_4)_2(OH)_6.3H_2O$, are both single locality mineral species occurring at the same deposit, notably lacking significant solid solution between Pb and Ca in their reported analyses (Strunz and Tennyson, 1967; this study; Frondel and Strunz, 1960). If unbonded lone pair electrons belonging to Pb in fleischerite disrupt the centrosymmetry seen in schaurteite, this would explain an ostensibly limited solid solution between fleischerite and schaurteite.

Previous studies of fleischerite group minerals noted relatively large displacement parameters for O atoms in the $SO_4$ tetrahedron. For this reason, Otto (1975) proposed a split site for the O1 atom in the structure of synthetic fleischerite. When Barkley *et al.* (2011) reported the structure of the isotypic $Mn^{4+}$ analog despujolsite, they also noted large displacement parameters for O1. However, Barkley *et al.* (2011) proposed a single O1 site for despujolsite after an analysis of the displacement parameters demonstrated that the $SO_4$ group behaves as a rigid body with significant translation (0.72 Å) and libration (7.95°). Using translation-libration-screw motion (TLS) modelling software (Downs, 2000), the $SO_4$ group in schaurteite similarly shows rigid body behavior with 0.73 Å of translation and 7.97° of libration.

Consequently, this study proposes a single O1 atom model for schaurteite (Figure 4).

## Experimental

The schaurteite specimen used in this study came from the Tsumeb Corporation mine, Tsumeb, Otavi Mountains, Namibia and remains on deposition (sample R120104) with the RRUFF project (http://www.rruff.info). Schaurteite forms colorless fibrous crystals in a matrix of quartz, calcite, and germanite.

Chemical analyses were performed on a Cameca SX-100 electron microprobe at the Lunar and Planetary Laboratory, University of Arizona. The electron microprobe sample and the single-crystal fragment came from the same parent sample. Like despujolsite (Barkley *et al.* 2011), schaurteite was fugitive under the electron beam, leading to the choice of the following operating conditions: 20 kV exciting voltage, 6 nA operating current, and a spot size of 5 microns. The average of 13 analyses gave $GeO_2$ 17.97%, CaO 30.41%, and $SO_3$ 29.22%. Normalizing to 17 O atoms (which includes 6 moles $H_2O$ per formula unit), the combined empirical and structural chemical formula becomes $Ca_{3.01}Ge_{0.95}(S_{2.03}O_8)(OH)_6.3H_2O$. Further details of the electron microprobe analysis and formula calculations are available on the RRUFF web site (http://www.rruff.info/R120104).

## Refinement

To model possible variable occupancy of cations, site occupancies were allowed to vary without restraints. The results justified a model with full occupancies of Ca, Ge, and S, corroborated by electron microprobe data showing only these elements (with $Z > 8$). Two hydrogen atom positions were refined without restraints, both with reasonable isotropic displacement parameters.

## Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: XtalDraw (Downs & Hall-Wallace, 2003); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

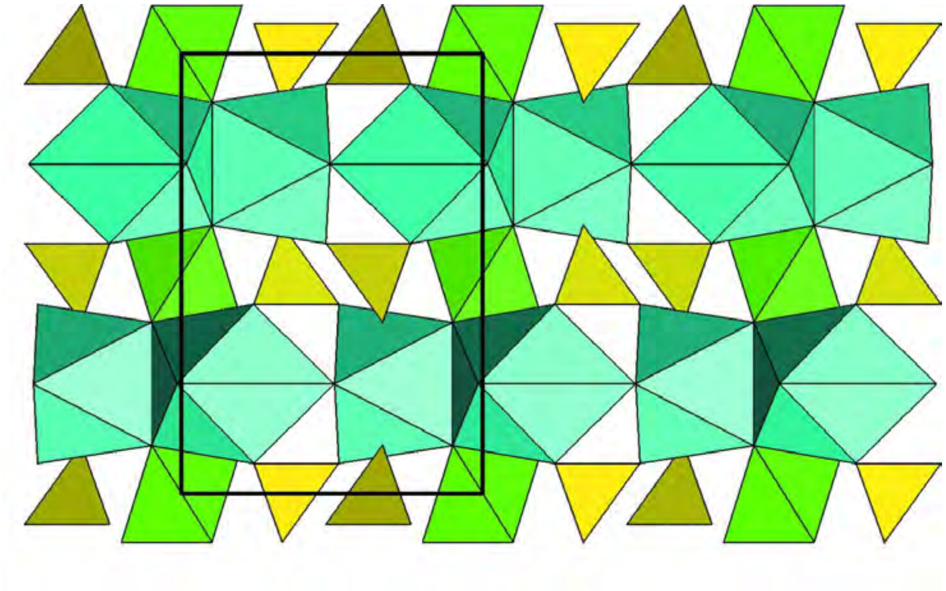

**Figure 1**

Polyhedral view of the schaurteite structure down [100], with slabs of light blue $Ca(OH)_4O_2(H_2O)_2$ polyhedra, interleaved with a mixed layer of green $Ge(OH)_6$ octahedra and yellow $SO_4$ tetrahedra. Unit cell outline shown in black.

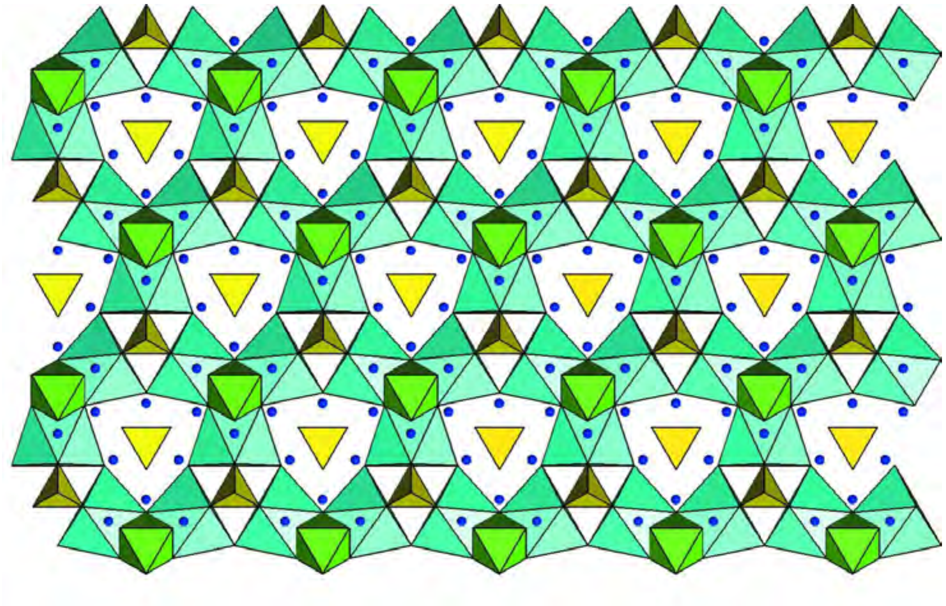

**Figure 2**

Polyhedral view of the schaurteite structure down [001], showing a single layer of light blue $Ca(OH)_4O_2(H_2O)_2$ polyhedra, a single mixed layer of green $Ge(OH)_6$ octahedra and yellow $SO_4$ tetrahedra, and dark blue H atoms in both layers.

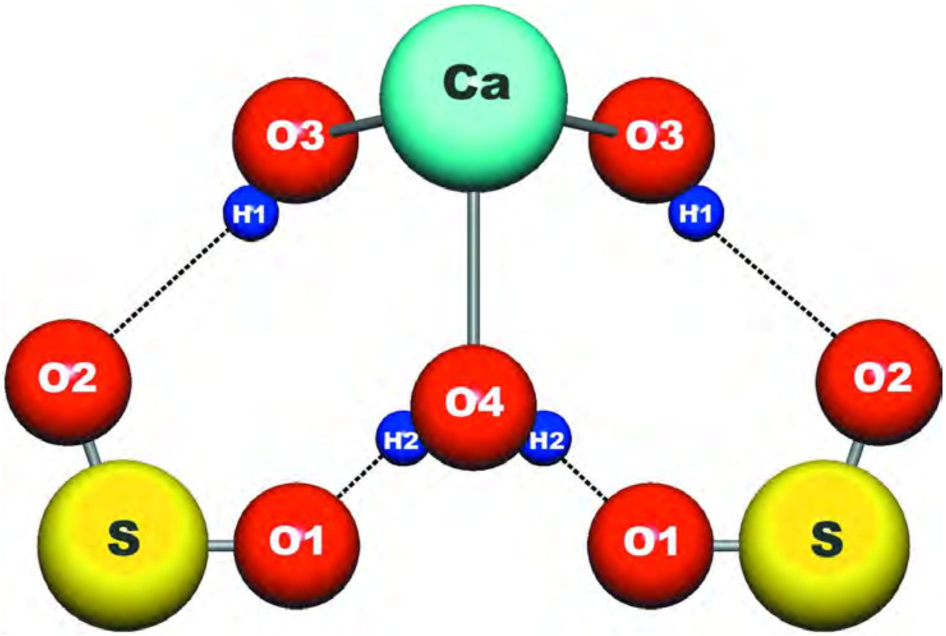

**Figure 3**

Hydrogen bonding in schaurteite, showing O4—H2···O1 at 2.04 Å and O3—H1···O2 at 2.12 Å.

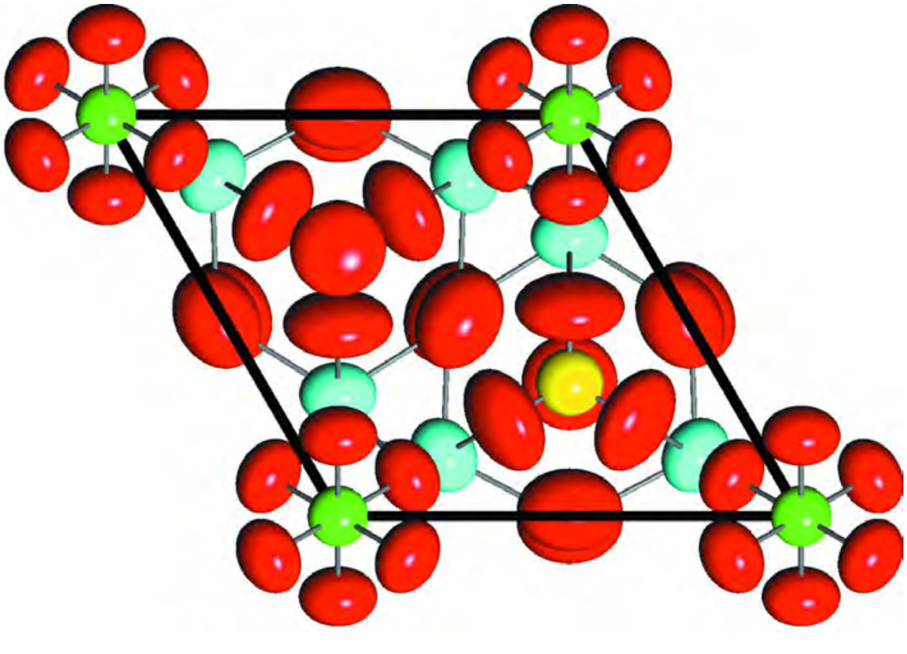

**Figure 4**

Ellipsoidal view of the schaurteite structure down [001], showing red O atoms, yellow S atoms, green Ge atoms, and light blue Ca atoms. Unit cell outline shown in black. The large circular ellipsoid at [2/3,1/3,*z*] represents the O1 atom (3 m. symmetry), which forms the apex of a rigid $SO_4$ tetrahedron with significant translation (0.73 Å) and libration (7.97°).

## Tricalcium germanium bis(sulfate) hexahydroxide trihydrate

*Crystal data*

$Ca_3Ge(SO_4)_2(OH)_6(H_2O)_3$
$M_r$ = 541.05
Hexagonal, $P6_3/mmc$
Hall symbol: -P 6c 2c
$a$ = 8.5253 (4) Å
$c$ = 10.8039 (6) Å
$V$ = 680.03 (6) Å$^3$
$Z$ = 2
$F$(000) = 544
$D_x$ = 2.642 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2603 reflections
$\theta$ = 2.8–28.0°
$\mu$ = 3.79 mm$^{-1}$
$T$ = 296 K
Hexagonal prism section, colourless
0.05 × 0.03 × 0.03 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
$T_{min}$ = 0.656, $T_{max}$ = 0.747
17243 measured reflections
536 independent reflections
456 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061
$\theta_{max}$ = 33.1°, $\theta_{min}$ = 2.8°
$h = -10 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.045
$S$ = 1.15
536 reflections
35 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0131P)^2 + 0.5886P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ge | 0.0000 | 0.0000 | 0.0000 | 0.00762 (11) |
| Ca | 0.30387 (8) | 0.15193 (4) | 0.2500 | 0.01107 (12) |
| S | 0.3333 | 0.6667 | 0.52599 (7) | 0.00963 (16) |
| O1 | 0.3333 | 0.6667 | 0.1106 (2) | 0.0167 (5) |
| O2 | 0.4786 (2) | 0.23930 (11) | 0.06925 (14) | 0.0190 (3) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.10006 (10) | 0.2001 (2) | 0.10982 (13) | 0.0106 (3) |
| O4 | 0.50772 (16) | 0.49228 (16) | 0.7500 | 0.0190 (5) |
| H1 | 0.142 (2) | 0.284 (4) | 0.075 (2) | 0.028 (8)* |
| H2 | 0.543 (2) | 0.457 (2) | 0.695 (3) | 0.051 (11)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ge | 0.00878 (15) | 0.00878 (15) | 0.0053 (2) | 0.00439 (7) | 0.000 | 0.000 |
| Ca | 0.0098 (3) | 0.0131 (2) | 0.0091 (2) | 0.00491 (13) | 0.000 | 0.000 |
| S | 0.0108 (2) | 0.0108 (2) | 0.0073 (3) | 0.00538 (11) | 0.000 | 0.000 |
| O1 | 0.0217 (9) | 0.0217 (9) | 0.0067 (11) | 0.0109 (4) | 0.000 | 0.000 |
| O2 | 0.0114 (7) | 0.0243 (7) | 0.0169 (7) | 0.0057 (4) | 0.0039 (6) | 0.0020 (3) |
| O3 | 0.0131 (5) | 0.0086 (7) | 0.0087 (6) | 0.0043 (3) | −0.0004 (3) | −0.0008 (5) |
| O4 | 0.0239 (9) | 0.0239 (9) | 0.0143 (10) | 0.0158 (10) | 0.000 | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ge—O3 | 1.8949 (14) | Ca—O3$^{iii}$ | 2.4890 (9) |
| Ge—O3$^{i}$ | 1.8949 (14) | Ca—O3$^{vii}$ | 2.4890 (9) |
| Ge—O3$^{ii}$ | 1.8949 (14) | Ca—O4$^{viii}$ | 2.6284 (12) |
| Ge—O3$^{iii}$ | 1.8949 (14) | Ca—O4$^{ix}$ | 2.6284 (12) |
| Ge—O3$^{iv}$ | 1.8949 (14) | S—O2$^{x}$ | 1.4651 (16) |
| Ge—O3$^{v}$ | 1.8949 (14) | S—O2$^{xi}$ | 1.4651 (16) |
| Ca—O2 | 2.3404 (15) | S—O2$^{xii}$ | 1.4651 (16) |
| Ca—O2$^{vi}$ | 2.3404 (15) | S—O1$^{vi}$ | 1.475 (3) |
| Ca—O3 | 2.4890 (9) | O3—H1 | 0.73 (3) |
| Ca—O3$^{vi}$ | 2.4890 (9) | O4—H2 | 0.79 (3) |
| | | | |
| O3—Ge—O3$^{i}$ | 180.0 | O2—Ca—O3$^{vii}$ | 147.24 (3) |
| O3—Ge—O3$^{ii}$ | 95.05 (6) | O2$^{vi}$—Ca—O3$^{vii}$ | 79.95 (4) |
| O3$^{i}$—Ge—O3$^{ii}$ | 84.95 (6) | O3—Ca—O3$^{vii}$ | 105.61 (6) |
| O3—Ge—O3$^{iii}$ | 84.95 (6) | O3$^{vi}$—Ca—O3$^{vii}$ | 61.87 (7) |
| O3$^{i}$—Ge—O3$^{iii}$ | 95.05 (6) | O3$^{iii}$—Ca—O3$^{vii}$ | 74.96 (5) |
| O3$^{ii}$—Ge—O3$^{iii}$ | 180.00 (10) | O2—Ca—O4$^{viii}$ | 73.04 (3) |
| O3—Ge—O3$^{iv}$ | 95.05 (6) | O2$^{vi}$—Ca—O4$^{viii}$ | 73.04 (3) |
| O3$^{i}$—Ge—O3$^{iv}$ | 84.95 (6) | O3—Ca—O4$^{viii}$ | 83.33 (5) |
| O3$^{ii}$—Ge—O3$^{iv}$ | 84.95 (6) | O3$^{vi}$—Ca—O4$^{viii}$ | 83.33 (5) |
| O3$^{iii}$—Ge—O3$^{iv}$ | 95.05 (6) | O3$^{iii}$—Ca—O4$^{viii}$ | 139.12 (3) |
| O3—Ge—O3$^{v}$ | 84.95 (6) | O3$^{vii}$—Ca—O4$^{viii}$ | 139.12 (3) |
| O3$^{i}$—Ge—O3$^{v}$ | 95.05 (6) | O2—Ca—O4$^{ix}$ | 73.04 (3) |
| O3$^{ii}$—Ge—O3$^{v}$ | 95.05 (6) | O2$^{vi}$—Ca—O4$^{ix}$ | 73.04 (3) |
| O3$^{iii}$—Ge—O3$^{v}$ | 84.95 (6) | O3—Ca—O4$^{ix}$ | 139.12 (3) |
| O3$^{iv}$—Ge—O3$^{v}$ | 180.00 (14) | O3$^{vi}$—Ca—O4$^{ix}$ | 139.12 (3) |
| O2—Ca—O2$^{vi}$ | 113.10 (8) | O3$^{iii}$—Ca—O4$^{ix}$ | 83.33 (5) |
| O2—Ca—O3 | 79.95 (4) | O3$^{vii}$—Ca—O4$^{ix}$ | 83.33 (5) |
| O2$^{vi}$—Ca—O3 | 147.24 (3) | O4$^{viii}$—Ca—O4$^{ix}$ | 116.09 (10) |
| O2—Ca—O3$^{vi}$ | 147.24 (3) | O2—Ca—Ge | 73.16 (4) |
| O2$^{vi}$—Ca—O3$^{vi}$ | 79.95 (4) | O2$^{x}$—S—O2$^{xi}$ | 110.32 (7) |
| O3—Ca—O3$^{vi}$ | 74.96 (5) | O2$^{x}$—S—O2$^{xii}$ | 110.32 (7) |

| | | | |
|---|---|---|---|
| O2—Ca—O3$^{iii}$ | 79.95 (4) | O2$^{xi}$—S—O2$^{xii}$ | 110.32 (7) |
| O2$^{vi}$—Ca—O3$^{iii}$ | 147.24 (3) | O2$^{x}$—S—O1$^{vi}$ | 108.61 (7) |
| O3—Ca—O3$^{iii}$ | 61.87 (7) | O2$^{xi}$—S—O1$^{vi}$ | 108.60 (7) |
| O3$^{vi}$—Ca—O3$^{iii}$ | 105.61 (6) | O2$^{xii}$—S—O1$^{vi}$ | 108.60 (7) |

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*−*y*, *x*, −*z*; (iii) −*x*+*y*, −*x*, *z*; (iv) *y*, −*x*+*y*, −*z*; (v) −*y*, *x*−*y*, *z*; (vi) *x*, *y*, −*z*+1/2; (vii) −*x*+*y*, −*x*, −*z*+1/2; (viii) −*x*+1, −*y*+1, −*z*+1; (ix) *y*, −*x*+*y*, −*z*+1; (x) *y*, −*x*+*y*+1, *z*+1/2; (xi) −*x*+1, −*y*+1, *z*+1/2; (xii) *x*−*y*, *x*, *z*+1/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H1···O2$^{xiii}$ | 0.73 (3) | 2.12 (3) | 2.823 (2) | 164 (3) |
| O4—H2···O1$^{xiv}$ | 0.79 (3) | 2.04 (3) | 2.789 (2) | 158 (3) |

Symmetry codes: (xiii) *y*, *x*, −*z*; (xiv) *y*, −*x*+*y*, *z*+1/2.