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High-pressure synthesis and crystal structure of $SrGa_4As_4$

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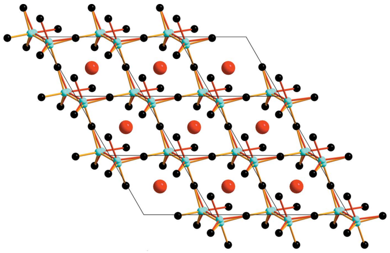
Strontium tetragallate(II,III) tetraarsenide, $SrGa_4As_4$, was synthesized in a Walker-type multianvil apparatus under high-pressure/high-temperature conditions of 8 GPa and 1573 K. The compound crystallizes in a new structure type ($P3_221$, $Z = 3$) as a three-dimensional (3D) framework of corner-sharing $SrAs_8$ quadratic antiprisms with strontium situated on a twofold rotation axis (Wyckoff position 3*b*). This arrangement is surrounded by a 3D framework which can be described as alternately stacked layers of either condensed $Ga^{III}As_4$ tetrahedra or honeycomb-like layers built up from distorted ethane-like $Ga^{II}{}_2As_6$ units comprising Ga—Ga bonds.

1. Chemical context

The ternary systems *A*–*Tr*–As (*A* = Ca, Sr or Ba; *Tr* = Ga or In) contain numerous compounds with different crystal structures based on $TrAs_4$ tetrahedra which occur isolated (Kauzlarich & Kuromoto, 1991), as dimers, as chains (Stoyko *et al.*, 2015; He *et al.*, 2012), condensed to ethane-like Tr_2As_6 groups (Mathieu *et al.*, 2008; Goforth *et al.*, 2009; He *et al.*, 2011) or as large supertetrahedral units (Weippert *et al.*, 2019). $SrGa_4As_4$ is the first high-pressure compound in this system and contains an unprecedented layer-like framework, thus expanding the structural variety of the *A*–*Tr*–As family.

2. Structural commentary

$SrGa_4As_4$ crystallizes in the space group $P3_221$ (No. 154) and constitutes a new structure type. Strontium is coordinated in a quadratic antiprismatic manner by eight As atoms (Fig. 1). The antiprisms are slightly distorted, with their quadratic planes twisted by ∼34° relative to each other instead of 45° for an ideal quadratic antiprism. Sr—As distances range from 3.2665 (4) to 3.4560 (4) Å. The $SrAs_8$ polyhedra are connected through common corners, each As atom shared by two quadratic antiprisms, building up a three-dimensional (3D) framework. A similar structural motif is known for $RbAg_2SbS_4$, which crystallizes in the space group $P3_121$ (Schimek *et al.*, 1996). The surrounding construct in the two crystal structures differs however. $SrGa_4As_4$ contains a 3D Ga/As framework that can be subdivided into two types of layers with an *AB* stacking sequence along the *c* axis. The first type is built up from corner- and edge-sharing $GaAs_4$ tetrahedra forming sheets with triangular voids (Fig. 2). The tetrahedra are distorted, with angles in the range of 100.790 (19)–127.996 (19)°, and have typical Ga—As distances of 2.4384 (5)–2.5470 (5) Å. The second layer type consists of distorted ethane-like Ga_2As_6 groups with nearly eclipsed conformations. The Ga_2As_6 groups are connected *via* common



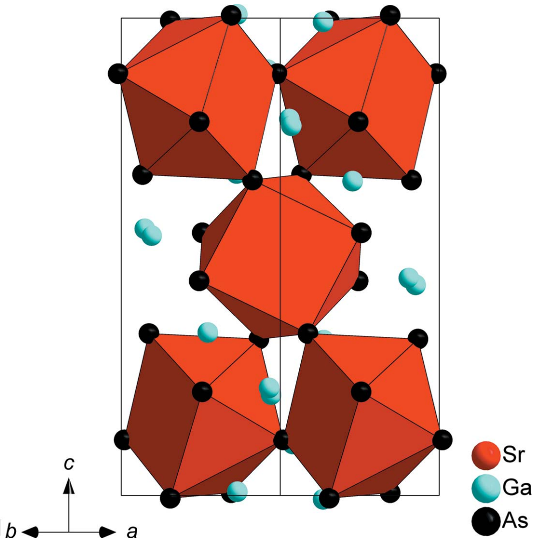


Figure 1
The unit cell of $SrGa_4As_4$, viewed along $[\overline{11}0]$, with the quadratic antiprismatic strontium coordination spheres shown as red polyhedra.

corners, forming a honeycomb-like sheet (Fig. 3). The Ga1*A* and Ga1*B* positions of the Ga–Ga dumbbell are disordered and were treated with split positions having an occupancy of 50% each (Fig. 4). The coordination of each of these Ga sites consists of three As atoms and one Ga atom forming trigonal pyramids, showing torsion angles of 114.5 (1)° for As1$^{\rm vi}$—Ga1*A*—Ga1*A*$^{\rm i}$—As1$^{\rm iv}$ and 119.3 (1)° for As2$^{\rm v}$—Ga1*B*—Ga1*B*$^{\rm i}$—As2$^{\rm vii}$ (for symmetry codes, see Fig. 4). The Ga—Ga distances range between 2.542 (8) and 2.572 (8) Å and are considered as Ga—Ga bonds, which is consistent with a charge-neutral compound. Ga—As distances between 2.477 (4) and 2.694 (2) Å for Ga1*A* are near to the covalent radii sum of 2.46 Å (Pauling, 1960). In comparison, the trigonal pyramid around Ga1*B* is elongated, with Ga—As distances of 2.415 (4)–2.845 (2) Å.

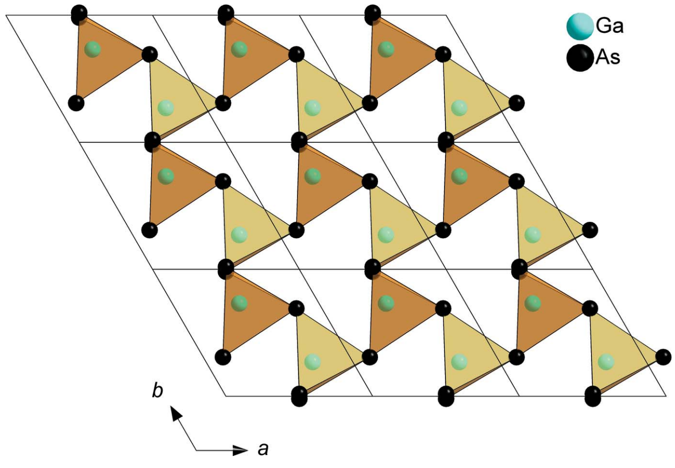


Figure 2
Edge- and corner-sharing $GaAs_4$ tetrahedra forming a layer with triangular voids viewed along [001].

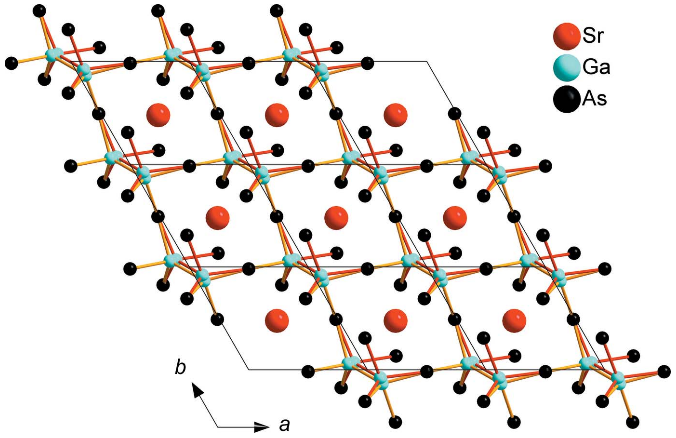


Figure 3
Corner-sharing Ga_2As_6 dumbbells with disordered Ga positions forming a honeycomb-like layer viewed along [001].

3. Synthesis and crystallization

The starting material SrAs was synthesized by heating stoichiometric amounts of Sr (Sigma–Aldrich, 99.95%) and As (Alfa Aesar, 99.99999+%) in alumina crucibles, sealed in silica ampules under an atmosphere of purified argon for 20 h at 1223 K. The title compound was obtained *via* high-pressure synthesis using a modified Walker-type multianvil set-up driven by a 1000 t hydraulic press (Voggenreiter, Mainleus, Germany). A Cr_2O_3-substituted (6%) MgO octahedron (Ceramic Substrates & Components, Isle of Wight, UK) with an edge length of 18 mm, housing a ZrO_2 sleeve with graphite sleeves (Schunk, Heuchelheim, Germany) for heating and a h-BN crucible (Henze, Kempten, Germany), was compressed with tungsten carbide cubes (Hawedia, Marklkofen, Germany) with an edge length of 11 mm. The starting mate-

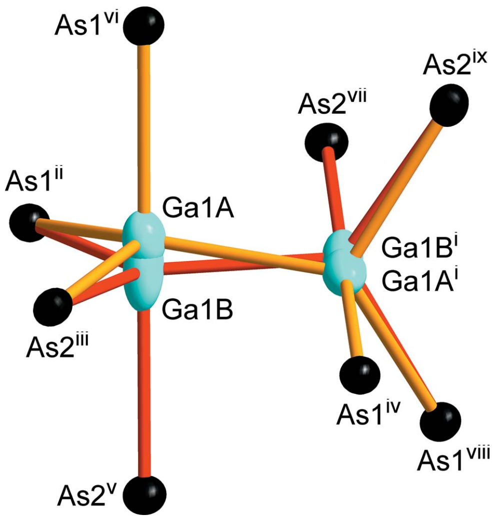


Figure 4
Ga_2As_6 groups with disordered Ga positions having an occupancy of 50%. Displacement ellipsoids are drawn at the 95% probability level. [Symmetry codes: (i) $-x + 2, -x + y + 1, -z + \frac{5}{3}$; (ii) $y, x, -z + 1$; (iii) $x, y + 1, z + 1$; (iv) $y + 1, x + 1, -z + 1$; (v) $y + 1, x, -z + 1$; (vi) $-y + 1, x - y + 1$ $z + \frac{2}{3}$; (vii) $-y + 1, x - y, z + \frac{2}{3}$; (viii) $-y + 2, x - y + 1, z + \frac{2}{3}$; (ix) $-x + 2, -x + y + 2, -z + \frac{2}{3}$.]

rials SrAs (73.4 mg, 0.452 mmol), Ga (66.5 mg, 0.953 mmol, Alfa Aesar, 99.999%) and As (60.1 mg, 0.802 mmol) were mixed in a glove-box (H_2O, O_2 <1 ppm) and filled into the octahedron assembly. The reaction was carried out at 8 GPa and 1573 K, with a dwell time of 3 h. The temperature was increased and decreased over a period of 1 h. The assembly was opened in a glove-box, revealing crystals with a metallic luster.

The composition of $SrGa_4As_4$ was verified by EDX measurements using a a Carl Zeiss EVO-MA 10 instrument with a Bruker Nano EDX detector. The experimental values [Sr 12 (1) at%, Ga 44 (2) at% and As 45 (1) at%] are in excellent agreement with the expected values (Sr 11.1 at%, Ga 44.4 at% and As 44.4 at%) within the typical error of the method, and confirm the composition obtained from single-crystal X-ray diffraction data.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The Ga1*A* and Ga1*B* positions were introduced as half-occupied split positions since one fully occupied position with a prolate ellipsoid caused residual densities in the order of 2.2 e Å^{-3}. Upon exclusion of the Ga1*A*/Ga1*B* positions, the contour difference map in *PLATON* (Spek, 2009) shows two clearly separated maxima justifying this approach. Structural data were standardized with *STRUCTURE-TIDY* (Gelato & Parthé, 1987).

Table 1
Experimental details.

Crystal data	
Chemical formula	$SrGa_4As_4$
M_r	666.18
Crystal system, space group	Trigonal, $P3_221$
Temperature (K)	293
a, *c* (Å)	6.3615 (1), 16.5792 (2)
V (Å^3)	581.05 (2)
Z	3
Radiation type	Mo *Kα*
μ (mm^{-1})	37.42
Crystal size (mm)	0.10 × 0.05 × 0.05
Data collection	
Diffractometer	Bruker APEXII D8 Quest CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.446, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14966, 928, 918
R_{int}	0.034
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.657
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.012, 0.025, 1.17
No. of reflections	928
No. of parameters	52
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.69
Absolute structure	Flack *x* determined using 340 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.024 (11)

Computer programs: *SAINT* (Bruker, 2016), *APEX3* (Bruker, 2016), *SUPERFLIP* (Palatinus & Chapuis, 2007), *EDMA* (Palatinus *et al.*, 2012), *SHELXL* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2014) and *PLATON* (Spek, 2009).

Acknowledgements

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References

Brandenburg, K. (2014). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (2016). *SAINT*, *APEX3* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.

Goforth, A. M., Hope, H., Condron, C. L., Kauzlarich, S. M., Jensen, N., Klavins, P., MaQuilon, S. & Fisk, Z. (2009). *Chem. Mater.* **21**, 4480–4489.

He, H., Stearrett, R., Nowak, E. R. & Bobev, S. (2011). *Eur. J. Inorg. Chem.* **2011**, 4025–4036.

He, H., Tyson, C., Saito, M. & Bobev, S. (2012). *J. Solid State Chem.* **188**, 59–65.

Kauzlarich, S. M. & Kuromoto, T. Y. (1991). *Croat. Chem. Acta*, **64**, 343–352.

Mathieu, J., Achey, R., Park, J., Purcell, K. M., Tozer, S. W. & Latturner, S. E. (2008). *Chem. Mater.* **20**, 5675–5681.

Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.

Palatinus, L., Prathapa, S. J. & van Smaalen, S. (2012). *J. Appl. Cryst.* **45**, 575–580.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Pauling, L. (1960). In The Nature of the Chemical Bond, 3rd ed. Ithaca: Cornell University Press.

Schimek, G. L., Pennington, W. T., Wood, P. T. & Kolis, J. W. (1996). *J. Solid State Chem.* **123**, 277–284.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Stoyko, S., Voss, L., He, H. & Bobev, S. (2015). *Crystals*, **5**, 433–446.

Weippert, V., Haffner, A., Stamatopoulos, A. & Johrendt, D. (2019). *J. Am. Chem. Soc.* **141**, 11245–11252.

supporting information

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Computing details

Data collection: *SAINT* (Bruker, 2016); cell refinement: *APEX3* (Bruker, 2016); data reduction: *APEX3* (Bruker, 2016); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007) and EDMA (Palatinus *et al.*, 2012); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2014); software used to prepare material for publication: *PLATON* (Spek, 2009).

Strontium tetragallate(II,III) tetraarsenide

Crystal data

$SrGa_4As_4$
$M_r = 666.18$
Trigonal, $P3_221$
$a = 6.3615\ (1)$ Å
$c = 16.5792\ (2)$ Å
$V = 581.05\ (2)$ Å^3
$Z = 3$
$F(000) = 882$
$D_x = 5.711$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9912 reflections
$\theta = 3.7$–$30.4°$
$\mu = 37.42$ mm^{-1}
$T = 293$ K
Block, black
0.10 × 0.05 × 0.05 mm

Data collection

Bruker APEXII D8 Quest CCD diffractometer
Radiation source: Iμ S
Goebel Mirror monochromator
combined φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.446$, $T_{max} = 0.746$
14966 measured reflections
928 independent reflections
918 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.7°$
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.012$
$wR(F^2) = 0.025$
$S = 1.17$
928 reflections
52 parameters
0 restraints
Primary atom site location: iterative
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0102P)^2 + 0.3943P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}
Absolute structure: Flack x determined using 340 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.024 (11)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr1	0.52374 (8)	0.000000	0.166667	0.01264 (11)	
Ga1A	0.8090 (7)	0.9427 (8)	0.8779 (2)	0.0120 (4)	0.5
Ga1B	0.8516 (7)	0.9303 (8)	0.8920 (2)	0.0175 (5)	0.5
Ga2	0.27470 (8)	0.54448 (7)	0.00800 (2)	0.00988 (9)	
As1	0.50915 (7)	0.49019 (6)	0.11634 (2)	0.00817 (8)	
As2	0.86593 (6)	0.17439 (6)	0.00577 (2)	0.00838 (8)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01406 (18)	0.0121 (2)	0.0111 (2)	0.00605 (12)	0.00104 (9)	0.00209 (17)
Ga1A	0.0136 (10)	0.0079 (6)	0.0131 (10)	0.0044 (6)	0.0032 (6)	0.0001 (6)
Ga1B	0.0184 (13)	0.0080 (7)	0.0206 (13)	0.0025 (7)	0.0107 (9)	−0.0018 (8)
Ga2	0.0105 (2)	0.00988 (18)	0.01119 (18)	0.00654 (16)	−0.00233 (16)	−0.00109 (14)
As1	0.00767 (16)	0.00801 (17)	0.00862 (16)	0.00376 (14)	−0.00032 (13)	0.00041 (12)
As2	0.00712 (16)	0.00890 (17)	0.00970 (17)	0.00444 (14)	0.00033 (13)	0.00055 (13)

Geometric parameters (Å, º)

Sr1—As2	3.2665 (4)	Ga1A—As1^{xii}	2.477 (4)
Sr1—As2^{i}	3.2666 (4)	Ga1A—As2^{xiii}	2.503 (4)
Sr1—As1^{i}	3.2739 (4)	Ga1A—Ga1B^{xiv}	2.5444 (13)
Sr1—As1	3.2739 (4)	Ga1A—Ga1A^{xiv}	2.572 (8)
Sr1—As1^{ii}	3.3048 (4)	Ga1A—As1^{xv}	2.694 (2)
Sr1—As1^{iii}	3.3048 (4)	Ga1B—As2^{xiii}	2.415 (4)
Sr1—Ga1B^{iv}	3.312 (4)	Ga1B—As1^{xii}	2.515 (4)
Sr1—Ga1B^{v}	3.312 (4)	Ga1B—Ga1B^{xiv}	2.542 (8)
Sr1—Ga1A^{vi}	3.346 (4)	Ga1B—As2^{xvi}	2.845 (2)
Sr1—Ga1A^{vii}	3.346 (4)	Ga2—As2^{viii}	2.4384 (5)
Sr1—Ga2^{viii}	3.3505 (4)	Ga2—As1	2.4668 (5)
Sr1—Ga2^{ix}	3.3506 (4)	Ga2—As2^{xvii}	2.4868 (5)
Sr1—As2^{x}	3.4560 (4)	Ga2—As1^{viii}	2.5470 (5)
Sr1—As2^{xi}	3.4560 (4)	Ga2—Ga2^{viii}	2.9844 (8)

As2—Sr1—As2^{i}	120.45 (2)	Ga1A^{xiv}—Ga1B—As2^{xvi}	89.08 (12)
As2—Sr1—As1^{i}	134.533 (8)	As2^{xiii}—Ga1B—Sr1^{xviii}	142.90 (10)
As2^{i}—Sr1—As1^{i}	78.453 (9)	As1^{xii}—Ga1B—Sr1^{xviii}	67.51 (9)
As2—Sr1—As1	78.453 (9)	Ga1B^{xiv}—Ga1B—Sr1^{xviii}	67.43 (7)
As2^{i}—Sr1—As1	134.533 (8)	Ga1A^{xiv}—Ga1B—Sr1^{xviii}	72.45 (15)

As1$^{\rm i}$—Sr1—As1	119.39 (2)
As2—Sr1—As1$^{\rm ii}$	79.285 (11)
As2$^{\rm i}$—Sr1—As1$^{\rm ii}$	74.128 (11)
As1$^{\rm i}$—Sr1—As1$^{\rm ii}$	66.217 (5)
As1—Sr1—As1$^{\rm ii}$	150.471 (11)
As2—Sr1—As1$^{\rm iii}$	74.128 (11)
As2$^{\rm i}$—Sr1—As1$^{\rm iii}$	79.284 (11)
As1$^{\rm i}$—Sr1—As1$^{\rm iii}$	150.470 (11)
As1—Sr1—As1$^{\rm iii}$	66.217 (5)
As1$^{\rm ii}$—Sr1—As1$^{\rm iii}$	124.89 (2)
As2—Sr1—Ga1B$^{\rm iv}$	51.25 (5)
As2$^{\rm i}$—Sr1—Ga1B$^{\rm iv}$	73.07 (5)
As1$^{\rm i}$—Sr1—Ga1B$^{\rm iv}$	109.71 (7)
As1—Sr1—Ga1B$^{\rm iv}$	126.49 (6)
As1$^{\rm ii}$—Sr1—Ga1B$^{\rm iv}$	44.67 (7)
As1$^{\rm iii}$—Sr1—Ga1B$^{\rm iv}$	81.77 (7)
As2—Sr1—Ga1B$^{\rm v}$	73.07 (5)
As2$^{\rm i}$—Sr1—Ga1B$^{\rm v}$	51.25 (5)
As1$^{\rm i}$—Sr1—Ga1B$^{\rm v}$	126.49 (6)
As1—Sr1—Ga1B$^{\rm v}$	109.71 (7)
As1$^{\rm ii}$—Sr1—Ga1B$^{\rm v}$	81.77 (7)
As1$^{\rm iii}$—Sr1—Ga1B$^{\rm v}$	44.67 (7)
Ga1B$^{\rm iv}$—Sr1—Ga1B$^{\rm v}$	45.14 (14)
As2—Sr1—Ga1A$^{\rm vi}$	111.75 (6)
As2$^{\rm i}$—Sr1—Ga1A$^{\rm vi}$	123.12 (5)
As1$^{\rm i}$—Sr1—Ga1A$^{\rm vi}$	48.02 (5)
As1—Sr1—Ga1A$^{\rm vi}$	74.76 (5)
As1$^{\rm ii}$—Sr1—Ga1A$^{\rm vi}$	95.97 (6)
As1$^{\rm iii}$—Sr1—Ga1A$^{\rm vi}$	138.60 (6)
Ga1B$^{\rm iv}$—Sr1—Ga1A$^{\rm vi}$	135.24 (5)
Ga1B$^{\rm v}$—Sr1—Ga1A$^{\rm vi}$	174.30 (10)
As2—Sr1—Ga1A$^{\rm vii}$	123.12 (5)
As2$^{\rm i}$—Sr1—Ga1A$^{\rm vii}$	111.75 (6)
As1$^{\rm i}$—Sr1—Ga1A$^{\rm vii}$	74.76 (5)
As1—Sr1—Ga1A$^{\rm vii}$	48.02 (5)
As1$^{\rm ii}$—Sr1—Ga1A$^{\rm vii}$	138.60 (6)
As1$^{\rm iii}$—Sr1—Ga1A$^{\rm vii}$	95.97 (7)
Ga1B$^{\rm iv}$—Sr1—Ga1A$^{\rm vii}$	174.30 (10)
Ga1B$^{\rm v}$—Sr1—Ga1A$^{\rm vii}$	135.23 (5)
Ga1A$^{\rm vi}$—Sr1—Ga1A$^{\rm vii}$	45.20 (14)
As2—Sr1—Ga2$^{\rm viii}$	43.223 (9)
As2$^{\rm i}$—Sr1—Ga2$^{\rm viii}$	161.548 (17)
As1$^{\rm i}$—Sr1—Ga2$^{\rm viii}$	118.760 (14)
As1—Sr1—Ga2$^{\rm viii}$	45.205 (10)
As1$^{\rm ii}$—Sr1—Ga2$^{\rm viii}$	105.550 (10)
As1$^{\rm iii}$—Sr1—Ga2$^{\rm viii}$	86.374 (9)
Ga1B$^{\rm iv}$—Sr1—Ga2$^{\rm viii}$	93.55 (5)
Ga1B$^{\rm v}$—Sr1—Ga2$^{\rm viii}$	110.30 (5)
As2$^{\rm xvi}$—Ga1B—Sr1$^{\rm xviii}$	63.55 (6)
As2$^{\rm xiii}$—Ga1B—Sr1$^{\rm xv}$	67.96 (9)
As1$^{\rm xii}$—Ga1B—Sr1$^{\rm xv}$	137.34 (9)
Ga1B$^{\rm xiv}$—Ga1B—Sr1$^{\rm xv}$	68.95 (7)
Ga1A$^{\rm xiv}$—Ga1B—Sr1$^{\rm xv}$	64.32 (16)
As2$^{\rm xvi}$—Ga1B—Sr1$^{\rm xv}$	119.38 (13)
Sr1$^{\rm xviii}$—Ga1B—Sr1$^{\rm xv}$	136.38 (13)
As2$^{\rm xiii}$—Ga1B—Sr1$^{\rm xix}$	100.06 (10)
As1$^{\rm xii}$—Ga1B—Sr1$^{\rm xix}$	39.58 (5)
Ga1B$^{\rm xiv}$—Ga1B—Sr1$^{\rm xix}$	118.30 (16)
Ga1A$^{\rm xiv}$—Ga1B—Sr1$^{\rm xix}$	125.48 (7)
As2$^{\rm xvi}$—Ga1B—Sr1$^{\rm xix}$	138.21 (12)
Sr1$^{\rm xviii}$—Ga1B—Sr1$^{\rm xix}$	101.86 (10)
Sr1$^{\rm xv}$—Ga1B—Sr1$^{\rm xix}$	98.42 (5)
As2$^{\rm xiii}$—Ga1B—Sr1$^{\rm xiii}$	30.22 (6)
As1$^{\rm xii}$—Ga1B—Sr1$^{\rm xiii}$	86.93 (10)
Ga1B$^{\rm xiv}$—Ga1B—Sr1$^{\rm xiii}$	155.24 (14)
Ga1A$^{\rm xiv}$—Ga1B—Sr1$^{\rm xiii}$	146.47 (15)
As2$^{\rm xvi}$—Ga1B—Sr1$^{\rm xiii}$	80.65 (8)
Sr1$^{\rm xviii}$—Ga1B—Sr1$^{\rm xiii}$	128.07 (9)
Sr1$^{\rm xv}$—Ga1B—Sr1$^{\rm xiii}$	93.16 (8)
Sr1$^{\rm xix}$—Ga1B—Sr1$^{\rm xiii}$	80.08 (6)
As2$^{\rm viii}$—Ga2—As1	127.996 (19)
As2$^{\rm viii}$—Ga2—As2$^{\rm xvii}$	101.790 (19)
As1—Ga2—As2$^{\rm xvii}$	107.308 (18)
As2$^{\rm viii}$—Ga2—As1$^{\rm viii}$	112.107 (18)
As1—Ga2—As1$^{\rm viii}$	100.790 (19)
As2$^{\rm xvii}$—Ga2—As1$^{\rm viii}$	104.987 (18)
As2$^{\rm viii}$—Ga2—Ga2$^{\rm viii}$	160.190 (16)
As1—Ga2—Ga2$^{\rm viii}$	54.718 (14)
As2$^{\rm xvii}$—Ga2—Ga2$^{\rm viii}$	94.821 (13)
As1$^{\rm viii}$—Ga2—Ga2$^{\rm viii}$	52.245 (14)
As2$^{\rm viii}$—Ga2—Sr1$^{\rm xx}$	66.554 (14)
As1—Ga2—Sr1$^{\rm xx}$	164.526 (19)
As2$^{\rm xvii}$—Ga2—Sr1$^{\rm xx}$	70.850 (14)
As1$^{\rm viii}$—Ga2—Sr1$^{\rm xx}$	65.805 (12)
Ga2$^{\rm viii}$—Ga2—Sr1$^{\rm xx}$	109.825 (18)
As2$^{\rm viii}$—Ga2—Sr1$^{\rm xxi}$	65.922 (13)
As1—Ga2—Sr1$^{\rm xxi}$	62.098 (13)
As2$^{\rm xvii}$—Ga2—Sr1$^{\rm xxi}$	126.697 (18)
As1$^{\rm viii}$—Ga2—Sr1$^{\rm xxi}$	128.043 (18)
Ga2$^{\rm viii}$—Ga2—Sr1$^{\rm xxi}$	112.066 (16)
Sr1$^{\rm xx}$—Ga2—Sr1$^{\rm xxi}$	131.844 (12)
As2$^{\rm viii}$—Ga2—Sr1$^{\rm xvii}$	94.008 (14)
As1—Ga2—Sr1$^{\rm xvii}$	87.434 (14)
As2$^{\rm xvii}$—Ga2—Sr1$^{\rm xvii}$	33.956 (10)
As1$^{\rm viii}$—Ga2—Sr1$^{\rm xvii}$	137.041 (15)
Ga2$^{\rm viii}$—Ga2—Sr1$^{\rm xvii}$	105.802 (10)

Ga1A^{vi}—Sr1—Ga2^{viii}	75.33 (5)
Ga1A^{vii}—Sr1—Ga2^{viii}	81.05 (6)
As2—Sr1—Ga2^{ix}	161.548 (17)
As2^{i}—Sr1—Ga2^{ix}	43.223 (9)
As1^{i}—Sr1—Ga2^{ix}	45.205 (10)
As1—Sr1—Ga2^{ix}	118.759 (14)
As1^{ii}—Sr1—Ga2^{ix}	86.374 (9)
As1^{iii}—Sr1—Ga2^{ix}	105.549 (10)
Ga1B^{iv}—Sr1—Ga2^{ix}	110.30 (5)
Ga1B^{v}—Sr1—Ga2^{ix}	93.55 (5)
Ga1A^{vi}—Sr1—Ga2^{ix}	81.05 (6)
Ga1A^{vii}—Sr1—Ga2^{ix}	75.33 (5)
Ga2^{viii}—Sr1—Ga2^{ix}	154.42 (2)
As2—Sr1—As2^{x}	69.230 (6)
As2^{i}—Sr1—As2^{x}	150.543 (8)
As1^{i}—Sr1—As2^{x}	76.839 (11)
As1—Sr1—As2^{x}	72.738 (10)
As1^{ii}—Sr1—As2^{x}	81.367 (9)
As1^{iii}—Sr1—As2^{x}	129.115 (8)
Ga1B^{iv}—Sr1—As2^{x}	100.60 (6)
Ga1B^{v}—Sr1—As2^{x}	140.87 (6)
Ga1A^{vi}—Sr1—As2^{x}	43.14 (7)
Ga1A^{vii}—Sr1—As2^{x}	76.71 (7)
Ga2^{viii}—Sr1—As2^{x}	42.823 (9)
Ga2^{ix}—Sr1—As2^{x}	120.222 (14)
As2—Sr1—As2^{xi}	150.543 (8)
As2^{i}—Sr1—As2^{xi}	69.230 (6)
As1^{i}—Sr1—As2^{xi}	72.738 (10)
As1—Sr1—As2^{xi}	76.839 (11)
As1^{ii}—Sr1—As2^{xi}	129.114 (8)
As1^{iii}—Sr1—As2^{xi}	81.366 (9)
Ga1B^{iv}—Sr1—As2^{xi}	140.87 (6)
Ga1B^{v}—Sr1—As2^{xi}	100.60 (6)
Ga1A^{vi}—Sr1—As2^{xi}	76.71 (7)
Ga1A^{vii}—Sr1—As2^{xi}	43.14 (7)
Ga2^{viii}—Sr1—As2^{xi}	120.222 (14)
Ga2^{ix}—Sr1—As2^{xi}	42.823 (9)
As2^{x}—Sr1—As2^{xi}	117.382 (19)
As1^{xii}—Ga1A—As2^{xiii}	114.84 (16)
As1^{xii}—Ga1A—Ga1B^{xiv}	119.2 (2)
As2^{xiii}—Ga1A—Ga1B^{xiv}	121.43 (16)
As1^{xii}—Ga1A—Ga1A^{xiv}	127.04 (14)
As2^{xiii}—Ga1A—Ga1A^{xiv}	112.61 (17)
Ga1B^{xiv}—Ga1A—Ga1A^{xiv}	8.82 (9)
As1^{xii}—Ga1A—As1^{xv}	87.94 (10)
As2^{xiii}—Ga1A—As1^{xv}	107.20 (13)
Ga1B^{xiv}—Ga1A—As1^{xv}	95.81 (13)
Ga1A^{xiv}—Ga1A—As1^{xv}	99.49 (15)
Sr1^{xx}—Ga2—Sr1^{xvii}	97.358 (11)
Sr1^{xxi}—Ga2—Sr1^{xvii}	93.202 (9)
As2^{viii}—Ga2—Sr1	154.513 (14)
As1—Ga2—Sr1	29.480 (10)
As2^{xvii}—Ga2—Sr1	84.221 (13)
As1^{viii}—Ga2—Sr1	89.655 (14)
Ga2^{viii}—Ga2—Sr1	37.413 (11)
Sr1^{xx}—Ga2—Sr1	137.673 (13)
Sr1^{xxi}—Ga2—Sr1	90.483 (9)
Sr1^{xvii}—Ga2—Sr1	77.087 (5)
As2^{viii}—Ga2—Sr1^{xxii}	123.013 (14)
As1—Ga2—Sr1^{xxii}	78.871 (13)
As2^{xvii}—Ga2—Sr1^{xxii}	117.500 (15)
As1^{viii}—Ga2—Sr1^{xxii}	22.713 (10)
Ga2^{viii}—Ga2—Sr1^{xxii}	37.772 (10)
Sr1^{xx}—Ga2—Sr1^{xxii}	88.357 (8)
Sr1^{xxi}—Ga2—Sr1^{xxii}	111.288 (14)
Sr1^{xvii}—Ga2—Sr1^{xxii}	141.184 (8)
Sr1—Ga2—Sr1^{xxii}	73.220 (6)
Ga2—As1—Ga1A^{xii}	114.64 (6)
Ga2—As1—Ga1B^{xii}	105.91 (6)
Ga1A^{xii}—As1—Ga1B^{xii}	9.02 (9)
Ga2—As1—Ga2^{viii}	73.038 (18)
Ga1A^{xii}—As1—Ga2^{viii}	96.32 (10)
Ga1B^{xii}—As1—Ga2^{viii}	96.14 (9)
Ga2—As1—Ga1A^{vii}	98.03 (9)
Ga1A^{xii}—As1—Ga1A^{vii}	141.90 (4)
Ga1B^{xii}—As1—Ga1A^{vii}	147.27 (17)
Ga2^{viii}—As1—Ga1A^{vii}	112.22 (9)
Ga2—As1—Sr1	128.755 (16)
Ga1A^{xii}—As1—Sr1	102.71 (6)
Ga1B^{xii}—As1—Sr1	111.12 (6)
Ga2^{viii}—As1—Sr1	68.989 (12)
Ga1A^{vii}—As1—Sr1	67.39 (9)
Ga2—As1—Sr1^{xxi}	76.628 (13)
Ga1A^{xii}—As1—Sr1^{xxi}	73.33 (8)
Ga1B^{xii}—As1—Sr1^{xxi}	67.82 (8)
Ga2^{viii}—As1—Sr1^{xxi}	139.977 (16)
Ga1A^{vii}—As1—Sr1^{xxi}	97.23 (9)
Sr1—As1—Sr1^{xxi}	150.472 (11)
Ga2—As1—Sr1^{xvii}	65.908 (13)
Ga1A^{xii}—As1—Sr1^{xvii}	161.16 (10)
Ga1B^{xii}—As1—Sr1^{xvii}	156.82 (8)
Ga2^{viii}—As1—Sr1^{xvii}	101.547 (13)
Ga1A^{vii}—As1—Sr1^{xvii}	32.12 (9)
Sr1—As1—Sr1^{xvii}	89.333 (9)
Sr1^{xxi}—As1—Sr1^{xvii}	89.018 (12)
Ga1B^{xxiii}—As2—Ga2^{viii}	109.16 (6)

As1^{xii}—Ga1A—Sr1^{xv}	151.81 (10)
As2^{xiii}—Ga1A—Sr1^{xv}	70.77 (10)
Ga1B^{xiv}—Ga1A—Sr1^{xv}	72.42 (16)
Ga1A^{xiv}—Ga1A—Sr1^{xv}	67.40 (7)
As1^{xv}—Ga1A—Sr1^{xv}	64.59 (7)
As1^{xii}—Ga1A—Sr1^{xviii}	64.22 (9)
As2^{xiii}—Ga1A—Sr1^{xviii}	128.43 (8)
Ga1B^{xiv}—Ga1A—Sr1^{xviii}	63.92 (16)
Ga1A^{xiv}—Ga1A—Sr1^{xviii}	68.55 (7)
As1^{xv}—Ga1A—Sr1^{xviii}	123.83 (13)
Sr1^{xv}—Ga1A—Sr1^{xviii}	135.95 (13)
As1^{xii}—Ga1A—Sr1^{xix}	44.97 (5)
As2^{xiii}—Ga1A—Sr1^{xix}	105.82 (11)
Ga1B^{xiv}—Ga1A—Sr1^{xix}	127.80 (7)
Ga1A^{xiv}—Ga1A—Sr1^{xix}	135.48 (17)
As1^{xv}—Ga1A—Sr1^{xix}	46.51 (6)
Sr1^{xv}—Ga1A—Sr1^{xix}	107.02 (6)
Sr1^{xviii}—Ga1A—Sr1^{xix}	104.00 (10)
As1^{xii}—Ga1A—Sr1^{xiii}	85.55 (10)
As2^{xiii}—Ga1A—Sr1^{xiii}	29.68 (6)
Ga1B^{xiv}—Ga1A—Sr1^{xiii}	149.64 (10)
Ga1A^{xiv}—Ga1A—Sr1^{xiii}	140.99 (16)
As1^{xv}—Ga1A—Sr1^{xiii}	102.85 (10)
Sr1^{xv}—Ga1A—Sr1^{xiii}	94.16 (9)
Sr1^{xviii}—Ga1A—Sr1^{xiii}	120.80 (7)
Sr1^{xix}—Ga1A—Sr1^{xiii}	81.80 (6)
As2^{xiii}—Ga1B—As1^{xii}	116.66 (16)
As2^{xiii}—Ga1B—Ga1B^{xiv}	125.23 (17)
As1^{xii}—Ga1B—Ga1B^{xiv}	117.83 (16)
As2^{xiii}—Ga1B—Ga1A^{xiv}	116.7 (2)
As1^{xii}—Ga1B—Ga1A^{xiv}	126.56 (18)
Ga1B^{xiv}—Ga1B—Ga1A^{xiv}	8.90 (9)
As2^{xiii}—Ga1B—As2^{xvi}	80.20 (9)
As1^{xii}—Ga1B—As2^{xvi}	102.75 (11)
Ga1B^{xiv}—Ga1B—As2^{xvi}	93.10 (15)
Ga1B^{xxiii}—As2—Ga2^{xxiv}	107.80 (10)
Ga2^{viii}—As2—Ga2^{xxiv}	111.741 (17)
Ga1B^{xxiii}—As2—Ga1A^{xxiii}	8.97 (10)
Ga2^{viii}—As2—Ga1A^{xxiii}	100.47 (6)
Ga2^{xxiv}—As2—Ga1A^{xxiii}	110.18 (10)
Ga1B^{xxiii}—As2—Ga1B^{iv}	88.49 (12)
Ga2^{viii}—As2—Ga1B^{iv}	133.38 (9)
Ga2^{xxiv}—As2—Ga1B^{iv}	102.40 (9)
Ga1A^{xxiii}—As2—Ga1B^{iv}	96.31 (10)
Ga1B^{xxiii}—As2—Sr1	127.93 (10)
Ga2^{viii}—As2—Sr1	70.223 (14)
Ga2^{xxiv}—As2—Sr1	120.879 (15)
Ga1A^{xxiii}—As2—Sr1	128.03 (10)
Ga1B^{iv}—As2—Sr1	65.20 (9)
Ga1B^{xxiii}—As2—Sr1^{xxii}	71.67 (8)
Ga2^{viii}—As2—Sr1^{xxii}	73.974 (13)
Ga2^{xxiv}—As2—Sr1^{xxii}	66.325 (12)
Ga1A^{xxiii}—As2—Sr1^{xxii}	66.09 (8)
Ga1B^{iv}—As2—Sr1^{xxii}	151.44 (9)
Sr1—As2—Sr1^{xxii}	143.341 (12)
Ga1B^{xxiii}—As2—Sr1^{xxv}	21.56 (6)
Ga2^{viii}—As2—Sr1^{xxv}	128.411 (14)
Ga2^{xxiv}—As2—Sr1^{xxv}	103.930 (14)
Ga1A^{xxiii}—As2—Sr1^{xxv}	30.44 (6)
Ga1B^{iv}—As2—Sr1^{xxv}	68.27 (8)
Sr1—As2—Sr1^{xxv}	120.158 (9)
Sr1^{xxii}—As2—Sr1^{xxv}	88.418 (8)
Ga1B^{xxiii}—As2—Sr1^{xxvi}	139.37 (9)
Ga2^{viii}—As2—Sr1^{xxvi}	97.627 (13)
Ga2^{xxiv}—As2—Sr1^{xxvi}	32.041 (11)
Ga1A^{xxiii}—As2—Sr1^{xxvi}	142.22 (10)
Ga1B^{iv}—As2—Sr1^{xxvi}	94.88 (8)
Sr1—As2—Sr1^{xxvi}	89.306 (7)
Sr1^{xxii}—As2—Sr1^{xxvi}	87.812 (8)
Sr1^{xxv}—As2—Sr1^{xxvi}	130.398 (9)

Symmetry codes: (i) *x*−*y*, −*y*, −*z*+1/3; (ii) *x*, *y*−1, *z*; (iii) *x*−*y*+1, −*y*+1, −*z*+1/3; (iv) *y*, *x*−1, −*z*+1; (v) −*x*+*y*+1, −*x*+1, *z*−2/3; (vi) *y*−1, *x*−1, −*z*+1; (vii) −*x*+*y*, −*x*+1, *z*−2/3; (viii) *y*, *x*, −*z*; (ix) −*x*+*y*, −*x*, *z*+1/3; (x) *y*, *x*−1, −*z*; (xi) −*x*+*y*+1, −*x*+1, *z*+1/3; (xii) *y*, *x*, −*z*+1; (xiii) *x*, *y*+1, *z*+1; (xiv) −*x*+2, −*x*+*y*+1, −*z*+5/3; (xv) −*y*+1, *x*−*y*+1, *z*+2/3; (xvi) *y*+1, *x*, −*z*+1; (xvii) *x*−1, *y*, *z*; (xviii) −*y*+1, *x*−*y*, *z*+2/3; (xix) −*y*, *x*−*y*, *z*+2/3; (xx) −*y*, *x*−*y*, *z*−1/3; (xxi) *x*, *y*+1, *z*; (xxii) −*y*+1, *x*−*y*, *z*−1/3; (xxiii) *x*, *y*−1, *z*−1; (xxiv) *x*+1, *y*, *z*; (xxv) −*y*+1, *x*−*y*−1, *z*−1/3; (xxvi) *x*+1, *y*+1, *z*.