

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

The $P4_3$ enantiomorph of $\text{Sr}_2\text{As}_2\text{O}_7$ Aicha Mbarek^{a*} and Fadhila Edhokkar^b^aLaboratoire de Chimie Industrielle, Département de Génie des Matériaux, Ecole Nationale d'Ingénieurs de Sfax Université de Sfax, BP W3038, Sfax, Tunisia, and^bLaboratoire de l'Etat Solide, Faculté des Sciences, Université de Sfax, BP W3038, Sfax, Tunisia

Correspondence e-mail: mbarekaicha@yahoo.fr

Received 12 September 2013; accepted 19 November 2013

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{As}-\text{O}) = 0.004$ Å; R factor = 0.022; wR factor = 0.044; data-to-parameter ratio = 24.5.

The crystal structure of strontium diarsenate has been reinvestigated from single-crystal X-ray diffraction data. In contrast to the previous determinations of this structure [Weil *et al.* (2009). *Solid State Sci.* **11**, 2111–2117; Edhokkar *et al.* (2012). *Mater. Sci. Eng.*, **28**, 012017] and to all isotypic $A_2B_2O_7$ compounds that crystallize in the space group $P4_1$, the current redetermination revealed the $P4_3$ enantiomorph of $\text{Sr}_2\text{As}_2\text{O}_7$ with a purity of 96.3 (8)%. The crystal structure is made up from two eclipsed As_2O_7 diarsenate groups (symmetry 1) with characteristically longer As–O bridging bonds [1.756 (4)–1.781 (4) Å] than the terminal As–O bonds [1.636 (4)–1.679 (4) Å] and four Sr^{2+} sites with coordination numbers ranging from seven to nine. The building units are arranged in sheets parallel to (001).

Related literature

The crystal structure of $\text{Sr}_2\text{As}_2\text{O}_7$ has previously been refined from X-ray powder diffraction data (Weil *et al.*, 2009) in the space group $P4_1$ and was later reinvestigated (Edhokkar *et al.*, 2012). For isotypic structures crystallizing in space group $P4_1$, see: Baglio & Dann (1972); Webb (1966); Boudin *et al.* (1993); Müller-Bunz & Schleid (2000); Deng & Ibers (2005). For general structural features of the pyroarsenate anion, see: Weil & Stöger (2010).

Experimental

Crystal data

| | |
|------------------------------------|---|
| $\text{Sr}_2\text{As}_2\text{O}_7$ | $Z = 8$ |
| $M_r = 437.08$ | Mo $K\alpha$ radiation |
| Tetragonal, $P4_3$ | $\mu = 26.62 \text{ mm}^{-1}$ |
| $a = 7.1089$ (1) Å | $T = 296$ K |
| $c = 25.6160$ (4) Å | $0.75 \times 0.43 \times 0.14 \text{ mm}$ |
| $V = 1294.54$ (4) Å ³ | |

Data collection

| | |
|--|--|
| Bruker APEXII CCD diffractometer | 18524 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2008) | 4930 independent reflections |
| $T_{\min} = 0.448$, $T_{\max} = 0.751$ | 4593 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.035$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.022$ | $\Delta\rho_{\text{max}} = 0.92 \text{ e \AA}^{-3}$ |
| $wR(F^2) = 0.044$ | $\Delta\rho_{\text{min}} = -1.34 \text{ e \AA}^{-3}$ |
| $S = 1.01$ | Absolute structure: Flack (1983), 2400 Friedel pairs |
| 4930 reflections | Absolute structure parameter: 0.037 (8) |
| 201 parameters | |
| 1 restraint | |

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2013 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1999) and ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2770).

References

- Baglio, J. A. & Dann, J. N. (1972). *J. Solid State Chem.* **4**, 87–93.
- Boudin, S., Grandin, A., Borel, M. M., Leclaire, A. & Raveau, B. (1993). *Acta Cryst.* **C49**, 2062–2064.
- Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2008). *SADABS*, *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Deng, B. & Ibers, J. A. (2005). *Acta Cryst.* **E61**, i76–i78.
- Edhokkar, F., Hadrich, A., Graia, M. & Mhiri, T. (2012). *Mater. Sci. Eng.* **28**, 012017.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Müller-Bunz, H. & Schleid, T. (2000). *Z. Anorg. Allg. Chem.* **626**, 2549–2556.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Webb, N. C. (1966). *Acta Cryst.* **21**, 942–948.
- Weil, M., Dordevic, T., Lengauer, C. L. & Kolitsch, U. (2009). *Solid State Sci.* **11**, 2111–2117.
- Weil, M. & Stöger, B. (2010). *Acta Cryst.* **B66**, 603–614.

supporting information

Acta Cryst. (2013). E69, i84 [doi:10.1107/S1600536813031619]

The $P4_3$ enantiomorph of $\text{Sr}_2\text{As}_2\text{O}_7$

Aicha Mbarek and Fadhila Edhokkar

S1. Comment

The structure of strontium diarsenate, $\text{Sr}_2\text{As}_2\text{O}_7$, has previously been refined from X-ray powder diffraction data in the space group $P4_1$ using the Rietveld method (Weil *et al.*, 2009). The structure was later reinvestigated from single-crystal X-ray diffraction data in the same space group (Edhokkar *et al.*, 2012) and is isotypic with $\text{Sr}_2\text{V}_2\text{O}_7$ (Baglio & Dann, 1972), with $\text{Ce}_2\text{Si}_2\text{O}_7$ and its homologous lighter $\text{Ln}_2\text{Si}_2\text{O}_7$ lanthanides ($\text{Ln} = \text{La}, \text{Pr}, \text{Nd}, \text{Sm}$; Deng & Ibers, 2005), with the A -type structure of $\text{La}_2\text{Si}_2\text{O}_7$ (Müller-Bunz & Schleid, 2000) and with all of the β - $\text{Ca}_2\text{P}_2\text{O}_7$ -type structures (Webb, 1966; Boudin *et al.*, 1993).

We took the opportunity to have obtained single crystals of good quality of $\text{Sr}_2\text{As}_2\text{O}_7$ to improve the geometrical characteristics of this structure by a redetermination. Interestingly, it was found that in contrast to all above mentioned various $A_2B_2O_7$ structures (space group $P4_1$), the space group determined for the re-investigated material is $P4_3$, with only a minor contribution of 3.7 (8)% for the $P4_1$ enantiomorph. In comparison with the two previous studies, the precision in terms of bond lengths and angles is significantly higher for the current redetermination.

The structure of $\text{Sr}_2\text{As}_2\text{O}_7$ is characterized by the presence of two independent eclipsed As_2O_7 diarsenate groups, both with site symmetry 1 (Fig. 1). The As—O bridging bonds are characteristically longer (Weil & Stöger, 2010) than the terminal As—O bonds. The bridging As—O bonds range from 1.756 (4) to 1.781 (4) Å, the terminal bonds from 1.636 (4) to 1.679 (4) Å. This trend is also observed in the closely related structures of β - $\text{Ca}_2\text{P}_2\text{O}_7$ and $\text{Sr}_2\text{V}_2\text{O}_7$ but to a lesser extent in $\text{La}_2\text{Si}_2\text{O}_7$. This can be understood in terms of cationic repulsion since the $X^{5+}\cdots X^{5+}$ ($X = \text{P}, \text{As}, \text{V}$) repulsion is stronger than that of $\text{Si}^{4+}\cdots \text{Si}^{4+}$. The As—O—As bridging angles, *viz.* 126.8 (2)° and 129.3 (2)°, are slightly greater than the corresponding V—O—V angles, 123.04° and 123.53°, in $\text{Sr}_2\text{V}_2\text{O}_7$.

The crystal packing is based on discrete Sr^{2+} cations and isolated $(\text{As}_2\text{O}_7)^{4-}$ anions arranged in sheets parallel to (001) (Fig. 2). The Sr^{2+} cations are divided into four independent atomic sites and exhibit coordination numbers from seven to nine, with irregular coordination polyhedra and Sr—O distances spreading over the range 2.458 (4) - 3.228 (5) Å.

S2. Experimental

Single crystals of the title compound were synthesized in a solid state reaction by reacting As_2O_5 with SrCO_3 in an alumina boat. A mixture of these reagents in the molar ratio 30:70 was used for the synthesis. The mixture was heated at 823 K for 24 h. After grinding, the reacting mixture was heated up to 1173 K and maintained at this temperature for 48 h. Then the mixture was cooled to room temperature by switching off the furnace power. Translucent single crystals of $\text{Sr}_2\text{As}_2\text{O}_7$ were extracted from the batch.

S3. Refinement

Reflections (0 0 4), (0 0 $\bar{4}$), (0 1 2) and (0 1 1) were omitted from the refinement due to large differences between calculated and measured intensities. With regard to the anisotropic refinement of the atomic displacement parameters it

should be mentioned that a first attempt carried out from the initial data collection routinely recorded using an exposure time of 10 s per frame resulted in some large ADP max/min ratios and either prolate or oblate displacement ellipsoids for some oxygen atoms. The corresponding value of θ_{\max} for this data collection was 29.51° . Then a new data collection was carried out with an exposure time of 20 s per frame. The corresponding refinement lead to more homogeneous and acceptable values of the principal mean square atomic displacements U . For this data collection the θ_{\max} value was also increased up to 33.22° and resulted in 4593 intensities with $I > 2\sigma(I)$ versus 3324 in the preceding data collection. The highest residual peak in the final difference Fourier map was located 0.70 \AA from the Sr2 site and the deepest hole was located 0.65 \AA from the As4 site.

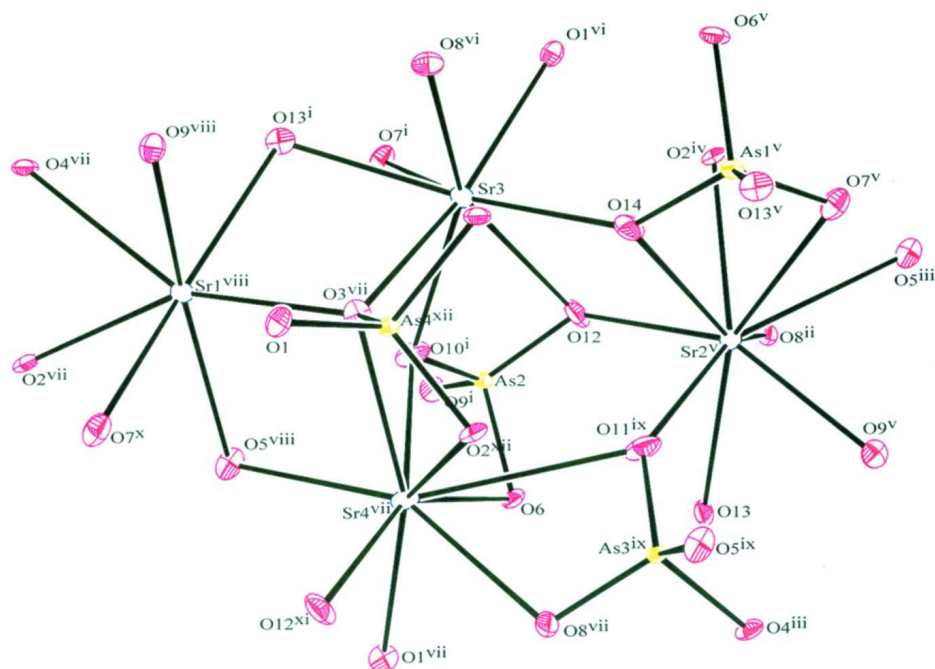
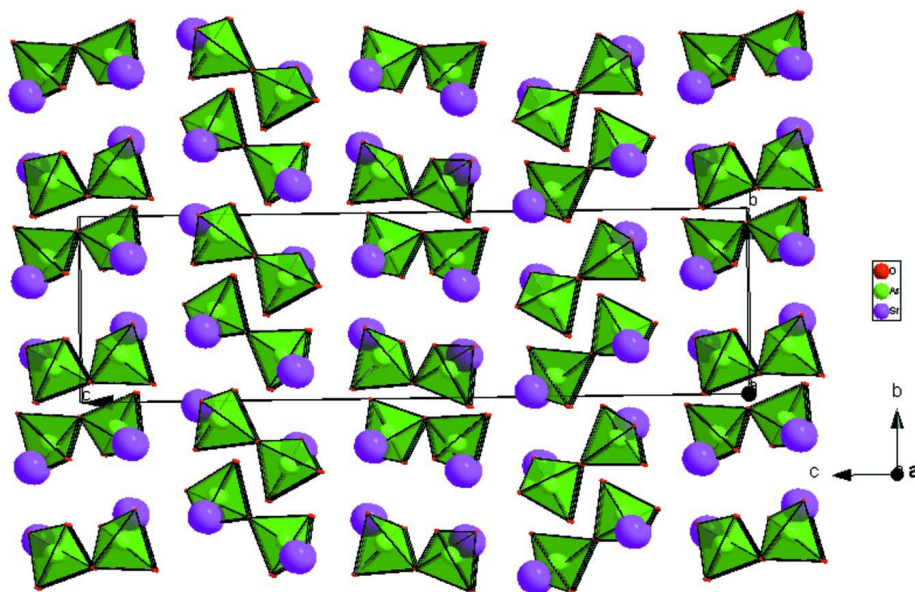


Figure 1

A view of a part of the structure of $\text{Sr}_2\text{As}_2\text{O}_7$. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $y, 1 - x, 1/4 + z$; (ii) $1 - y, x, 3/4 + z$; (iii) $1 - x, -y, 1/2 + z$; (iv) $1 - y, -1 + x, 3/4 + z$; (v) $y, -x, 1/4 + z$; (vi) $-y, x, 3/4 + z$; (vii) $x, y, 1 + z$; (viii) $-x, 1 - y, 1/2 + z$; (ix) $-x, -y, 1/2 + z$; (x) $-1 + y, 1 - x, 1/4 + z$; (xi) $-1 + x, y, z$; (xii) $-y, -1 + x, 3/4 + z$.]

**Figure 2**

Projection along [100] of the $\text{Sr}_2\text{As}_2\text{O}_7$ structure showing the stacking of $(\text{As}_2\text{O}_7)^{4-}$ sheets parallel to (001).

Strontium diarsenate

Crystal data

$\text{Sr}_2\text{As}_2\text{O}_7$

$M_r = 437.08$

Tetragonal, $P4_3$

$a = 7.1089 (1) \text{ \AA}$

$c = 25.6160 (4) \text{ \AA}$

$V = 1294.54 (4) \text{ \AA}^3$

$Z = 8$

$F(000) = 1584$

$D_x = 4.485 \text{ Mg m}^{-3}$

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

Cell parameters from 8103 reflections

$\theta = 3.3\text{--}33.2^\circ$

$\mu = 26.62 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.75 \times 0.43 \times 0.14 \text{ mm}$

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: $8.3333 \text{ pixels mm}^{-1}$

ω and φ scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.448$, $T_{\max} = 0.751$

18524 measured reflections

4930 independent reflections

4593 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 33.2^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -10 \rightarrow 10$

$k = -6 \rightarrow 10$

$l = -39 \rightarrow 39$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.044$

$S = 1.01$

4930 reflections

201 parameters

1 restraint

$$w = 1/[\sigma^2(F_o^2) + (0.0055P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.021$$

$$\Delta\rho_{\max} = 0.92 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.34 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL2013* (Sheldrick,

2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00348 (16)

Absolute structure: Flack (1983), 2400 Friedel pairs

Absolute structure parameter: 0.037 (8)

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. Refined as a 2-component inversion twin.

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|---------------|----------------------------------|
| Sr1 | 0.26434 (7) | 0.22687 (7) | 0.42638 (2) | 0.01083 (10) |
| Sr2 | 0.02701 (7) | 0.34822 (7) | 0.57318 (2) | 0.00890 (9) |
| Sr3 | 0.15408 (7) | 0.39584 (7) | 0.92865 (2) | 0.01120 (10) |
| Sr4 | 0.37469 (7) | 0.25769 (7) | 0.06464 (2) | 0.01125 (10) |
| As1 | 0.14561 (7) | 0.23414 (7) | 0.69696 (2) | 0.00774 (10) |
| As2 | 0.22057 (7) | 0.48276 (7) | 0.79885 (2) | 0.00756 (9) |
| As3 | 0.18673 (7) | 0.10525 (7) | 0.29124 (2) | 0.00678 (9) |
| As4 | 1.24906 (7) | 0.35443 (7) | 0.19001 (2) | 0.00640 (9) |
| O1 | 0.4586 (5) | 0.3299 (5) | -0.02876 (14) | 0.0127 (7) |
| O2 | 1.0936 (5) | 0.3899 (6) | 0.14240 (14) | 0.0126 (7) |
| O3 | 0.4187 (5) | 0.2147 (5) | 0.16739 (14) | 0.0109 (7) |
| O4 | 1.1085 (5) | 0.2261 (5) | 0.23449 (14) | 0.0113 (7) |
| O5 | 0.2999 (6) | 0.2626 (5) | 0.32782 (14) | 0.0139 (7) |
| O6 | 0.0777 (5) | 0.3681 (6) | 0.75140 (15) | 0.0127 (7) |
| O7 | 0.2725 (6) | 0.3751 (6) | 0.65898 (15) | 0.0152 (8) |
| O8 | 0.0556 (5) | 0.3427 (6) | 0.02051 (14) | 0.0121 (7) |
| O9 | 0.3251 (5) | 0.3037 (6) | 0.52047 (14) | 0.0129 (7) |
| O10 | 0.4811 (6) | 0.0546 (6) | 0.59334 (14) | 0.0163 (8) |
| O11 | 0.0026 (6) | 0.0009 (7) | 0.31632 (16) | 0.0189 (8) |
| O12 | 0.3813 (6) | 0.3334 (6) | 0.82115 (17) | 0.0182 (8) |
| O13 | 0.2817 (6) | 0.0576 (5) | 0.71776 (14) | 0.0122 (7) |
| O14 | 0.1680 (6) | 0.0503 (6) | 0.91819 (15) | 0.0156 (8) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|--------------|--------------|---------------|---------------|
| Sr1 | 0.0132 (2) | 0.0110 (2) | 0.00828 (19) | 0.00248 (18) | 0.00247 (16) | 0.00013 (16) |
| Sr2 | 0.0089 (2) | 0.0093 (2) | 0.00851 (18) | 0.00103 (17) | 0.00050 (15) | -0.00005 (16) |
| Sr3 | 0.0120 (2) | 0.0120 (2) | 0.00960 (19) | 0.00213 (18) | -0.00190 (17) | 0.00077 (16) |
| Sr4 | 0.0129 (2) | 0.0132 (2) | 0.00763 (18) | 0.00355 (19) | -0.00066 (16) | 0.00142 (16) |
| As1 | 0.0091 (2) | 0.0073 (2) | 0.0068 (2) | 0.00129 (19) | -0.00043 (16) | -0.00053 (16) |

| | | | | | | |
|-----|-------------|-------------|--------------|---------------|---------------|---------------|
| As2 | 0.0083 (2) | 0.0084 (2) | 0.00595 (19) | -0.00026 (19) | -0.00020 (17) | 0.00083 (17) |
| As3 | 0.0076 (2) | 0.0081 (2) | 0.00462 (19) | 0.00012 (18) | 0.00048 (16) | 0.00111 (16) |
| As4 | 0.0073 (2) | 0.0073 (2) | 0.00457 (18) | 0.00068 (18) | 0.00009 (15) | -0.00018 (16) |
| O1 | 0.0133 (18) | 0.0152 (19) | 0.0096 (15) | 0.0030 (15) | 0.0030 (13) | -0.0028 (14) |
| O2 | 0.0128 (18) | 0.0175 (19) | 0.0075 (15) | -0.0007 (16) | -0.0048 (13) | 0.0039 (14) |
| O3 | 0.0098 (17) | 0.0108 (17) | 0.0121 (16) | 0.0030 (14) | 0.0039 (13) | -0.0032 (13) |
| O4 | 0.0087 (17) | 0.0170 (18) | 0.0083 (15) | 0.0000 (15) | -0.0006 (12) | 0.0069 (13) |
| O5 | 0.020 (2) | 0.0112 (18) | 0.0101 (16) | -0.0031 (15) | -0.0064 (15) | -0.0013 (13) |
| O6 | 0.0123 (18) | 0.0159 (18) | 0.0098 (14) | 0.0029 (15) | -0.0020 (13) | -0.0076 (13) |
| O7 | 0.0156 (19) | 0.0155 (19) | 0.0146 (17) | 0.0006 (16) | 0.0049 (14) | 0.0042 (14) |
| O8 | 0.0122 (18) | 0.0149 (19) | 0.0092 (16) | -0.0041 (15) | -0.0006 (13) | 0.0011 (13) |
| O9 | 0.0101 (18) | 0.017 (2) | 0.0114 (16) | 0.0024 (15) | -0.0034 (13) | 0.0018 (14) |
| O10 | 0.026 (2) | 0.014 (2) | 0.0090 (17) | 0.0048 (17) | 0.0049 (15) | 0.0046 (13) |
| O11 | 0.0121 (19) | 0.027 (2) | 0.0178 (18) | -0.0041 (18) | 0.0026 (15) | 0.0114 (16) |
| O12 | 0.017 (2) | 0.0113 (19) | 0.026 (2) | 0.0025 (16) | -0.0098 (16) | 0.0051 (16) |
| O13 | 0.0158 (18) | 0.0089 (17) | 0.0120 (16) | 0.0037 (15) | -0.0005 (14) | 0.0017 (13) |
| O14 | 0.022 (2) | 0.0133 (19) | 0.0119 (17) | 0.0013 (16) | -0.0051 (14) | 0.0050 (14) |

Geometric parameters (Å, °)

| | | | |
|------------------------|------------|--------------------------|------------|
| Sr1—O9 | 2.509 (4) | As2—O12 | 1.661 (4) |
| Sr1—O5 | 2.550 (4) | As2—O6 | 1.781 (4) |
| Sr1—O13 ⁱ | 2.552 (4) | As2—Sr4 ^{viii} | 3.5090 (7) |
| Sr1—O3 ⁱⁱ | 2.555 (4) | As2—Sr1 ⁱⁱ | 3.6159 (7) |
| Sr1—O2 ⁱⁱ | 2.597 (4) | As2—Sr2 ⁱⁱ | 3.6547 (7) |
| Sr1—O7 ⁱⁱⁱ | 2.622 (4) | As2—Sr2 ^{iv} | 3.7874 (7) |
| Sr1—O4 ⁱⁱ | 2.824 (4) | As2—Sr4 ^{xiv} | 3.8092 (7) |
| Sr1—As4 ⁱⁱ | 3.4611 (7) | As3—O11 | 1.636 (4) |
| Sr1—As3 | 3.6106 (6) | As3—O5 | 1.666 (4) |
| Sr1—As2 ⁱⁱⁱ | 3.6159 (7) | As3—O8 ^{iv} | 1.679 (4) |
| Sr1—As1 ⁱ | 3.6288 (7) | As3—O4 ^{xiii} | 1.778 (4) |
| Sr1—As1 ⁱⁱⁱ | 3.6500 (8) | As3—Sr2 ⁱⁱⁱ | 3.4509 (7) |
| Sr2—O11 ^{iv} | 2.507 (4) | As3—Sr4 ^{iv} | 3.5007 (7) |
| Sr2—O9 | 2.533 (4) | As3—Sr3 ^{xii} | 3.7318 (7) |
| Sr2—O12 ⁱ | 2.573 (4) | As3—Sr4 ⁱⁱ | 3.7791 (7) |
| Sr2—O8 ^v | 2.644 (4) | As4—O1 ^{xv} | 1.654 (4) |
| Sr2—O2 ^{vi} | 2.710 (4) | As4—O2 | 1.665 (4) |
| Sr2—O14 ⁱ | 2.805 (4) | As4—O3 ^{xvi} | 1.666 (4) |
| Sr2—O13 ⁱ | 2.807 (4) | As4—O4 | 1.769 (4) |
| Sr2—O7 | 2.813 (4) | As4—Sr4 ^{xvi} | 3.4036 (7) |
| Sr2—O5 ⁱⁱ | 3.013 (4) | As4—Sr1 ⁱⁱⁱ | 3.4610 (7) |
| Sr2—As1 | 3.3796 (7) | As4—Sr3 ^{xvii} | 3.6580 (7) |
| Sr2—As3 ⁱⁱ | 3.4509 (7) | As4—Sr4 ^{xv} | 3.7288 (7) |
| Sr2—As2 ⁱⁱⁱ | 3.6547 (7) | As4—Sr3 ^{xviii} | 3.7738 (7) |
| Sr3—O10 ⁱⁱ | 2.458 (4) | As4—Sr1 ^{xix} | 3.7963 (7) |
| Sr3—O1 ^{vii} | 2.469 (4) | O1—As4 ^{xx} | 1.654 (4) |
| Sr3—O14 | 2.473 (4) | O1—Sr3 ^{xxi} | 2.469 (4) |
| Sr3—O8 ^{vii} | 2.484 (4) | O2—Sr1 ⁱⁱⁱ | 2.597 (4) |

| | | | |
|---|-------------|---|-------------|
| Sr3—O13 ⁱⁱ | 2.594 (4) | O2—Sr2 ^{xxii} | 2.710 (4) |
| Sr3—O3 ^{viii} | 2.643 (4) | O2—Sr4 ^{xvi} | 2.974 (4) |
| Sr3—O7 ⁱⁱ | 2.878 (4) | O3—As4 ^{xiii} | 1.666 (4) |
| Sr3—O12 | 3.223 (5) | O3—Sr1 ⁱⁱⁱ | 2.555 (4) |
| Sr3—As1 ⁱⁱ | 3.3422 (7) | O3—Sr3 ^{xii} | 2.643 (4) |
| Sr3—As2 | 3.4149 (7) | O4—As3 ^{xvi} | 1.778 (4) |
| Sr3—As4 ^{ix} | 3.6580 (7) | O4—Sr1 ⁱⁱⁱ | 2.824 (4) |
| Sr3—As3 ^{viii} | 3.7317 (7) | O5—Sr4 ⁱⁱ | 2.618 (4) |
| Sr4—O1 | 2.519 (4) | O5—Sr2 ⁱⁱⁱ | 3.013 (4) |
| Sr4—O10 ^x | 2.554 (4) | O6—Sr4 ^{viii} | 2.883 (4) |
| Sr4—O12 ^{xi} | 2.588 (4) | O7—Sr1 ⁱⁱ | 2.622 (4) |
| Sr4—O8 | 2.605 (4) | O7—Sr3 ⁱⁱⁱ | 2.878 (4) |
| Sr4—O5 ⁱⁱⁱ | 2.618 (4) | O8—As3 ⁱ | 1.679 (4) |
| Sr4—O3 | 2.668 (4) | O8—Sr3 ^{xxi} | 2.484 (4) |
| Sr4—O6 ^{xii} | 2.883 (4) | O8—Sr2 ^{xxiii} | 2.644 (4) |
| Sr4—O2 ^{xiii} | 2.974 (4) | O9—As2 ⁱⁱⁱ | 1.656 (4) |
| Sr4—O11 ⁱ | 3.228 (5) | O10—As2 ⁱⁱⁱ | 1.660 (4) |
| Sr4—As4 ^{xiii} | 3.4036 (7) | O10—Sr3 ⁱⁱⁱ | 2.458 (4) |
| Sr4—As3 ⁱ | 3.5006 (7) | O10—Sr4 ^{xxiv} | 2.554 (4) |
| Sr4—As2 ^{xii} | 3.5091 (7) | O11—Sr2 ⁱ | 2.507 (4) |
| As1—O14 ⁱ | 1.644 (4) | O11—Sr4 ^{iv} | 3.228 (5) |
| As1—O7 | 1.663 (4) | O12—Sr2 ^{iv} | 2.573 (4) |
| As1—O13 | 1.672 (4) | O12—Sr4 ^{xiv} | 2.588 (4) |
| As1—O6 | 1.756 (4) | O13—Sr1 ^{iv} | 2.552 (4) |
| As1—Sr3 ⁱⁱⁱ | 3.3422 (7) | O13—Sr3 ⁱⁱⁱ | 2.594 (4) |
| As1—Sr1 ^{iv} | 3.6288 (7) | O13—Sr2 ^{iv} | 2.807 (4) |
| As1—Sr1 ⁱⁱ | 3.6501 (8) | O14—As1 ^{iv} | 1.644 (4) |
| As2—O9 ⁱⁱ | 1.656 (4) | O14—Sr2 ^{iv} | 2.805 (4) |
| As2—O10 ⁱⁱ | 1.660 (4) | | |
| O9—Sr1—O5 | 155.84 (13) | O2 ^{xiii} —Sr4—As4 ^{xiii} | 29.29 (7) |
| O9—Sr1—O13 ⁱ | 73.87 (12) | O11 ⁱ —Sr4—As4 ^{xiii} | 83.33 (8) |
| O5—Sr1—O13 ⁱ | 119.01 (13) | O1—Sr4—As3 ⁱ | 95.60 (9) |
| O9—Sr1—O3 ⁱⁱ | 84.02 (12) | O10 ^x —Sr4—As3 ⁱ | 108.37 (10) |
| O5—Sr1—O3 ⁱⁱ | 79.99 (12) | O12 ^{xi} —Sr4—As3 ⁱ | 92.48 (9) |
| O13 ⁱ —Sr1—O3 ⁱⁱ | 76.29 (12) | O8—Sr4—As3 ⁱ | 27.21 (8) |
| O9—Sr1—O2 ⁱⁱ | 116.98 (12) | O5 ⁱⁱⁱ —Sr4—As3 ⁱ | 176.99 (8) |
| O5—Sr1—O2 ⁱⁱ | 73.83 (12) | O3—Sr4—As3 ⁱ | 105.46 (8) |
| O13 ⁱ —Sr1—O2 ⁱⁱ | 125.55 (13) | O6 ^{xii} —Sr4—As3 ⁱ | 76.63 (8) |
| O3 ⁱⁱ —Sr1—O2 ⁱⁱ | 151.94 (12) | O2 ^{xiii} —Sr4—As3 ⁱ | 60.36 (7) |
| O9—Sr1—O7 ⁱⁱⁱ | 88.17 (12) | O11 ⁱ —Sr4—As3 ⁱ | 27.77 (7) |
| O5—Sr1—O7 ⁱⁱⁱ | 73.88 (13) | As4 ^{xiii} —Sr4—As3 ⁱ | 86.271 (16) |
| O13 ⁱ —Sr1—O7 ⁱⁱⁱ | 158.20 (13) | O1—Sr4—As2 ^{xii} | 92.07 (9) |
| O3 ⁱⁱ —Sr1—O7 ⁱⁱⁱ | 89.87 (12) | O10 ^x —Sr4—As2 ^{xii} | 26.22 (8) |
| O2 ⁱⁱ —Sr1—O7 ⁱⁱⁱ | 73.47 (13) | O12 ^{xi} —Sr4—As2 ^{xii} | 173.16 (9) |
| O9—Sr1—O4 ⁱⁱ | 72.18 (12) | O8—Sr4—As2 ^{xii} | 111.43 (9) |
| O5—Sr1—O4 ⁱⁱ | 127.99 (11) | O5 ⁱⁱⁱ —Sr4—As2 ^{xii} | 84.85 (9) |
| O13 ⁱ —Sr1—O4 ⁱⁱ | 79.84 (12) | O3—Sr4—As2 ^{xii} | 88.69 (8) |

| | | | |
|--|--------------|---|--------------|
| O3 ⁱⁱ —Sr1—O4 ⁱⁱ | 150.11 (11) | O6 ^{xii} —Sr4—As2 ^{xii} | 30.39 (7) |
| O2 ⁱⁱ —Sr1—O4 ⁱⁱ | 57.93 (10) | O2 ^{xiii} —Sr4—As2 ^{xii} | 122.04 (8) |
| O7 ⁱⁱⁱ —Sr1—O4 ⁱⁱ | 106.75 (11) | O11 ⁱ —Sr4—As2 ^{xii} | 68.79 (8) |
| O9—Sr1—As4 ⁱⁱ | 94.82 (9) | As4 ^{xiii} —Sr4—As2 ^{xii} | 111.225 (17) |
| O5—Sr1—As4 ⁱⁱ | 100.31 (9) | As3 ⁱ —Sr4—As2 ^{xii} | 93.097 (17) |
| O13 ⁱ —Sr1—As4 ⁱⁱ | 105.86 (9) | O14 ⁱ —As1—O7 | 111.7 (2) |
| O3 ⁱⁱ —Sr1—As4 ⁱⁱ | 177.20 (8) | O14 ⁱ —As1—O13 | 114.7 (2) |
| O2 ⁱⁱ —Sr1—As4 ⁱⁱ | 27.46 (8) | O7—As1—O13 | 108.97 (19) |
| O7 ⁱⁱⁱ —Sr1—As4 ⁱⁱ | 87.54 (9) | O14 ⁱ —As1—O6 | 106.16 (19) |
| O4 ⁱⁱ —Sr1—As4 ⁱⁱ | 30.61 (7) | O7—As1—O6 | 106.7 (2) |
| O9—Sr1—As3 | 178.33 (9) | O13—As1—O6 | 108.23 (18) |
| O5—Sr1—As3 | 24.46 (9) | O14 ⁱ —As1—Sr3 ⁱⁱⁱ | 135.60 (14) |
| O13 ⁱ —Sr1—As3 | 107.32 (8) | O7—As1—Sr3 ⁱⁱⁱ | 59.43 (14) |
| O3 ⁱⁱ —Sr1—As3 | 97.39 (8) | O13—As1—Sr3 ⁱⁱⁱ | 49.64 (13) |
| O2 ⁱⁱ —Sr1—As3 | 61.39 (8) | O6—As1—Sr3 ⁱⁱⁱ | 118.15 (13) |
| O7 ⁱⁱⁱ —Sr1—As3 | 90.92 (9) | O14 ⁱ —As1—Sr2 | 55.72 (14) |
| O4 ⁱⁱ —Sr1—As3 | 106.77 (8) | O7—As1—Sr2 | 56.06 (15) |
| As4 ⁱⁱ —Sr1—As3 | 83.737 (15) | O13—As1—Sr2 | 128.58 (13) |
| O9—Sr1—As2 ⁱⁱⁱ | 23.60 (9) | O6—As1—Sr2 | 123.11 (13) |
| O5—Sr1—As2 ⁱⁱⁱ | 144.18 (9) | Sr3 ⁱⁱⁱ —As1—Sr2 | 98.775 (17) |
| O13 ⁱ —Sr1—As2 ⁱⁱⁱ | 95.02 (8) | O14 ⁱ —As1—Sr1 ^{iv} | 77.91 (15) |
| O3 ⁱⁱ —Sr1—As2 ⁱⁱⁱ | 99.15 (8) | O7—As1—Sr1 ^{iv} | 114.66 (14) |
| O2 ⁱⁱ —Sr1—As2 ⁱⁱⁱ | 96.26 (8) | O13—As1—Sr1 ^{iv} | 38.85 (13) |
| O7 ⁱⁱⁱ —Sr1—As2 ⁱⁱⁱ | 70.30 (9) | O6—As1—Sr1 ^{iv} | 133.52 (14) |
| O4 ⁱⁱ —Sr1—As2 ⁱⁱⁱ | 65.18 (8) | Sr3 ⁱⁱⁱ —As1—Sr1 ^{iv} | 70.007 (15) |
| As4 ⁱⁱ —Sr1—As2 ⁱⁱⁱ | 78.954 (15) | Sr2—As1—Sr1 ^{iv} | 97.921 (16) |
| As3—Sr1—As2 ⁱⁱⁱ | 154.799 (19) | O14 ⁱ —As1—Sr1 ⁱⁱ | 110.41 (15) |
| O9—Sr1—As1 ⁱ | 93.63 (9) | O7—As1—Sr1 ⁱⁱ | 40.61 (14) |
| O5—Sr1—As1 ⁱ | 104.86 (9) | O13—As1—Sr1 ⁱⁱ | 133.44 (14) |
| O13 ⁱ —Sr1—As1 ⁱ | 24.26 (8) | O6—As1—Sr1 ⁱⁱ | 68.19 (14) |
| O3 ⁱⁱ —Sr1—As1 ⁱ | 92.02 (8) | Sr3 ⁱⁱⁱ —As1—Sr1 ⁱⁱ | 89.525 (17) |
| O2 ⁱⁱ —Sr1—As1 ⁱ | 104.16 (9) | Sr2—As1—Sr1 ⁱⁱ | 70.709 (15) |
| O7 ⁱⁱⁱ —Sr1—As1 ⁱ | 177.52 (10) | Sr1 ^{iv} —As1—Sr1 ⁱⁱ | 155.19 (2) |
| O4 ⁱⁱ —Sr1—As1 ⁱ | 72.24 (8) | O9 ⁱⁱ —As2—O10 ⁱⁱ | 115.3 (2) |
| As4 ⁱⁱ —Sr1—As1 ⁱ | 90.599 (16) | O9 ⁱⁱ —As2—O12 | 115.6 (2) |
| As3—Sr1—As1 ⁱ | 87.242 (16) | O10 ⁱⁱ —As2—O12 | 110.6 (2) |
| As2 ⁱⁱⁱ —Sr1—As1 ⁱ | 110.953 (16) | O9 ⁱⁱ —As2—O6 | 106.33 (19) |
| O9—Sr1—As1 ⁱⁱⁱ | 74.19 (9) | O10 ⁱⁱ —As2—O6 | 97.71 (19) |
| O5—Sr1—As1 ⁱⁱⁱ | 93.54 (9) | O12—As2—O6 | 109.54 (19) |
| O13 ⁱ —Sr1—As1 ⁱⁱⁱ | 147.16 (8) | O9 ⁱⁱ —As2—Sr3 | 128.75 (13) |
| O3 ⁱⁱ —Sr1—As1 ⁱⁱⁱ | 107.70 (8) | O10 ⁱⁱ —As2—Sr3 | 42.37 (14) |
| O2 ⁱⁱ —Sr1—As1 ⁱⁱⁱ | 64.77 (9) | O12—As2—Sr3 | 69.19 (16) |
| O7 ⁱⁱⁱ —Sr1—As1 ⁱⁱⁱ | 24.38 (8) | O6—As2—Sr3 | 120.18 (14) |
| O4 ⁱⁱ —Sr1—As1 ⁱⁱⁱ | 83.36 (8) | O9 ⁱⁱ —As2—Sr4 ^{viii} | 125.22 (14) |
| As4 ⁱⁱ —Sr1—As1 ⁱⁱⁱ | 69.511 (15) | O10 ⁱⁱ —As2—Sr4 ^{viii} | 42.80 (14) |
| As3—Sr1—As1 ⁱⁱⁱ | 104.464 (16) | O12—As2—Sr4 ^{viii} | 119.14 (15) |
| As2 ⁱⁱⁱ —Sr1—As1 ⁱⁱⁱ | 52.204 (13) | O6—As2—Sr4 ^{viii} | 54.98 (13) |
| As1 ⁱ —Sr1—As1 ⁱⁱⁱ | 155.19 (2) | Sr3—As2—Sr4 ^{viii} | 73.384 (15) |

| | | | |
|--|-------------|---|--------------|
| O11 ^{iv} —Sr2—O9 | 84.28 (14) | O9 ⁱⁱ —As2—Sr1 ⁱⁱ | 37.32 (13) |
| O11 ^{iv} —Sr2—O12 ⁱ | 90.90 (14) | O10 ⁱⁱ —As2—Sr1 ⁱⁱ | 121.84 (15) |
| O9—Sr2—O12 ⁱ | 146.49 (13) | O12—As2—Sr1 ⁱⁱ | 127.42 (16) |
| O11 ^{iv} —Sr2—O8 ^v | 140.74 (13) | O6—As2—Sr1 ⁱⁱ | 69.06 (14) |
| O9—Sr2—O8 ^v | 91.02 (12) | Sr3—As2—Sr1 ⁱⁱ | 159.46 (2) |
| O12 ⁱ —Sr2—O8 ^v | 72.09 (13) | Sr4 ^{viii} —As2—Sr1 ⁱⁱ | 102.759 (16) |
| O11 ^{iv} —Sr2—O2 ^{vi} | 134.89 (12) | O9 ⁱⁱ —As2—Sr2 ⁱⁱ | 36.86 (13) |
| O9—Sr2—O2 ^{vi} | 134.38 (13) | O10 ⁱⁱ —As2—Sr2 ⁱⁱ | 84.95 (15) |
| O12 ⁱ —Sr2—O2 ^{vi} | 68.61 (12) | O12—As2—Sr2 ⁱⁱ | 112.34 (15) |
| O8 ^v —Sr2—O2 ^{vi} | 72.11 (11) | O6—As2—Sr2 ⁱⁱ | 133.96 (13) |
| O11 ^{iv} —Sr2—O14 ⁱ | 65.91 (12) | Sr3—As2—Sr2 ⁱⁱ | 92.341 (16) |
| O9—Sr2—O14 ⁱ | 124.71 (12) | Sr4 ^{viii} —As2—Sr2 ⁱⁱ | 115.447 (18) |
| O12 ⁱ —Sr2—O14 ⁱ | 82.20 (13) | Sr1 ⁱⁱ —As2—Sr2 ⁱⁱ | 70.779 (14) |
| O8 ^v —Sr2—O14 ⁱ | 141.14 (12) | O9 ⁱⁱ —As2—Sr2 ^{iv} | 140.88 (14) |
| O2 ^{vi} —Sr2—O14 ⁱ | 71.58 (12) | O10 ⁱⁱ —As2—Sr2 ^{iv} | 101.84 (16) |
| O11 ^{iv} —Sr2—O13 ⁱ | 75.47 (13) | O12—As2—Sr2 ^{iv} | 33.59 (15) |
| O9—Sr2—O13 ⁱ | 69.23 (11) | O6—As2—Sr2 ^{iv} | 79.11 (13) |
| O12 ⁱ —Sr2—O13 ⁱ | 77.44 (12) | Sr3—As2—Sr2 ^{iv} | 72.528 (14) |
| O8 ^v —Sr2—O13 ⁱ | 66.52 (11) | Sr4 ^{viii} —As2—Sr2 ^{iv} | 90.211 (16) |
| O2 ^{vi} —Sr2—O13 ⁱ | 132.64 (11) | Sr1 ⁱⁱ —As2—Sr2 ^{iv} | 127.992 (17) |
| O14 ⁱ —Sr2—O13 ⁱ | 135.72 (11) | Sr2 ⁱⁱ —As2—Sr2 ^{iv} | 145.57 (2) |
| O11 ^{iv} —Sr2—O7 | 99.69 (14) | O9 ⁱⁱ —As2—Sr4 ^{xiv} | 82.28 (14) |
| O9—Sr2—O7 | 84.60 (11) | O10 ⁱⁱ —As2—Sr4 ^{xiv} | 130.55 (14) |
| O12 ⁱ —Sr2—O7 | 128.84 (12) | O12—As2—Sr4 ^{xiv} | 33.36 (15) |
| O8 ^v —Sr2—O7 | 118.68 (12) | O6—As2—Sr4 ^{xiv} | 122.36 (12) |
| O2 ^{vi} —Sr2—O7 | 68.80 (12) | Sr3—As2—Sr4 ^{xiv} | 89.707 (16) |
| O14 ⁱ —Sr2—O7 | 58.30 (11) | Sr4 ^{viii} —As2—Sr4 ^{xiv} | 152.50 (2) |
| O13 ⁱ —Sr2—O7 | 153.66 (11) | Sr1 ⁱⁱ —As2—Sr4 ^{xiv} | 100.390 (16) |
| O11 ^{iv} —Sr2—O5 ⁱⁱ | 150.45 (13) | Sr2 ⁱⁱ —As2—Sr4 ^{xiv} | 86.127 (15) |
| O9—Sr2—O5 ⁱⁱ | 70.10 (12) | Sr2 ^{iv} —As2—Sr4 ^{xiv} | 63.658 (13) |
| O12 ⁱ —Sr2—O5 ⁱⁱ | 118.58 (12) | O11—As3—O5 | 118.0 (2) |
| O8 ^v —Sr2—O5 ⁱⁱ | 56.89 (11) | O11—As3—O8 ^{iv} | 110.1 (2) |
| O2 ^{vi} —Sr2—O5 ⁱⁱ | 65.15 (12) | O5—As3—O8 ^{iv} | 108.43 (19) |
| O14 ⁱ —Sr2—O5 ⁱⁱ | 116.99 (11) | O11—As3—O4 ^{xiii} | 106.86 (19) |
| O13 ⁱ —Sr2—O5 ⁱⁱ | 107.28 (10) | O5—As3—O4 ^{xiii} | 106.65 (18) |
| O7—Sr2—O5 ⁱⁱ | 64.40 (11) | O8 ^{iv} —As3—O4 ^{xiii} | 106.08 (17) |
| O11 ^{iv} —Sr2—As1 | 81.11 (10) | O11—As3—Sr2 ⁱⁱⁱ | 126.89 (15) |
| O9—Sr2—As1 | 105.15 (8) | O5—As3—Sr2 ⁱⁱⁱ | 60.81 (14) |
| O12 ⁱ —Sr2—As1 | 106.81 (10) | O8 ^{iv} —As3—Sr2 ⁱⁱⁱ | 48.13 (13) |
| O8 ^v —Sr2—As1 | 137.18 (8) | O4 ^{xiii} —As3—Sr2 ⁱⁱⁱ | 124.85 (12) |
| O2 ^{vi} —Sr2—As1 | 68.28 (8) | O11—As3—Sr4 ^{iv} | 66.80 (17) |
| O14 ⁱ —Sr2—As1 | 28.97 (8) | O5—As3—Sr4 ^{iv} | 119.24 (13) |
| O13 ⁱ —Sr2—As1 | 156.30 (8) | O8 ^{iv} —As3—Sr4 ^{iv} | 45.18 (13) |
| O7—Sr2—As1 | 29.36 (8) | O4 ^{xiii} —As3—Sr4 ^{iv} | 130.99 (13) |
| O5 ⁱⁱ —Sr2—As1 | 91.35 (7) | Sr2 ⁱⁱⁱ —As3—Sr4 ^{iv} | 70.382 (15) |
| O11 ^{iv} —Sr2—As3 ⁱⁱ | 161.51 (9) | O11—As3—Sr1 | 81.62 (15) |
| O9—Sr2—As3 ⁱⁱ | 81.87 (9) | O5—As3—Sr1 | 39.32 (14) |
| O12 ⁱ —Sr2—As3 ⁱⁱ | 93.90 (10) | O8 ^{iv} —As3—Sr1 | 111.43 (13) |

| | | | |
|---|--------------|---|--------------|
| O8 ^v —Sr2—As3 ⁱⁱ | 28.22 (8) | O4 ^{xiii} —As3—Sr1 | 135.74 (13) |
| O2 ^{vi} —Sr2—As3 ⁱⁱ | 63.13 (8) | Sr2 ⁱⁱⁱ —As3—Sr1 | 70.419 (14) |
| O14 ⁱ —Sr2—As3 ⁱⁱ | 132.45 (8) | Sr4 ^{iv} —As3—Sr1 | 92.705 (15) |
| O13 ⁱ —Sr2—As3 ⁱⁱ | 88.16 (8) | O11—As3—Sr3 ^{xii} | 113.46 (17) |
| O7—Sr2—As3 ⁱⁱ | 91.16 (8) | O5—As3—Sr3 ^{xii} | 125.02 (14) |
| O5 ⁱⁱ —Sr2—As3 ⁱⁱ | 28.88 (7) | O8 ^{iv} —As3—Sr3 ^{xii} | 32.45 (12) |
| As1—Sr2—As3 ⁱⁱ | 114.339 (17) | O4 ^{xiii} —As3—Sr3 ^{xii} | 74.41 (13) |
| O11 ^{iv} —Sr2—As2 ⁱⁱⁱ | 79.15 (11) | Sr2 ⁱⁱⁱ —As3—Sr3 ^{xii} | 73.859 (14) |
| O9—Sr2—As2 ⁱⁱⁱ | 23.09 (8) | Sr4 ^{iv} —As3—Sr3 ^{xii} | 66.010 (14) |
| O12 ⁱ —Sr2—As2 ⁱⁱⁱ | 165.61 (9) | Sr1—As3—Sr3 ^{xii} | 142.980 (19) |
| O8 ^v —Sr2—As2 ⁱⁱⁱ | 109.34 (8) | O11—As3—Sr4 ⁱⁱ | 119.22 (17) |
| O2 ^{vi} —Sr2—As2 ⁱⁱⁱ | 125.72 (9) | O5—As3—Sr4 ⁱⁱ | 35.87 (13) |
| O14 ⁱ —Sr2—As2 ⁱⁱⁱ | 102.79 (8) | O8 ^{iv} —As3—Sr4 ⁱⁱ | 128.93 (14) |
| O13 ⁱ —Sr2—As2 ⁱⁱⁱ | 89.91 (8) | O4 ^{xiii} —As3—Sr4 ⁱⁱ | 72.47 (13) |
| O7—Sr2—As2 ⁱⁱⁱ | 63.81 (8) | Sr2 ⁱⁱⁱ —As3—Sr4 ⁱⁱ | 89.553 (16) |
| O5 ⁱⁱ —Sr2—As2 ⁱⁱⁱ | 71.50 (8) | Sr4 ^{iv} —As3—Sr4 ⁱⁱ | 155.10 (2) |
| As1—Sr2—As2 ⁱⁱⁱ | 82.100 (15) | Sr1—As3—Sr4 ⁱⁱ | 66.002 (13) |
| As3 ⁱⁱ —Sr2—As2 ⁱⁱⁱ | 92.506 (17) | Sr3 ^{xii} —As3—Sr4 ⁱⁱ | 123.551 (17) |
| O10 ⁱⁱ —Sr3—O1 ^{vii} | 135.45 (13) | O1 ^{xv} —As4—O2 | 117.59 (19) |
| O10 ⁱⁱ —Sr3—O14 | 105.58 (13) | O1 ^{xv} —As4—O3 ^{xvi} | 113.31 (19) |
| O1 ^{vii} —Sr3—O14 | 79.88 (13) | O2—As4—O3 ^{xvi} | 108.41 (19) |
| O10 ⁱⁱ —Sr3—O8 ^{vii} | 144.63 (13) | O1 ^{xv} —As4—O4 | 107.41 (18) |
| O1 ^{vii} —Sr3—O8 ^{vii} | 78.44 (12) | O2—As4—O4 | 100.09 (18) |
| O14—Sr3—O8 ^{vii} | 87.88 (13) | O3 ^{xvi} —As4—O4 | 108.97 (18) |
| O10 ⁱⁱ —Sr3—O13 ⁱⁱ | 87.30 (13) | O1 ^{xv} —As4—Sr4 ^{xvi} | 121.83 (13) |
| O1 ^{vii} —Sr3—O13 ⁱⁱ | 103.23 (12) | O2—As4—Sr4 ^{xvi} | 60.90 (13) |
| O14—Sr3—O13 ⁱⁱ | 158.47 (13) | O3 ^{xvi} —As4—Sr4 ^{xvi} | 50.32 (13) |
| O8 ^{vii} —Sr3—O13 ⁱⁱ | 72.18 (12) | O4—As4—Sr4 ^{xvi} | 130.67 (13) |
| O10 ⁱⁱ —Sr3—O3 ^{viii} | 66.15 (12) | O1 ^{xv} —As4—Sr1 ⁱⁱⁱ | 122.48 (14) |
| O1 ^{vii} —Sr3—O3 ^{viii} | 158.40 (12) | O2—As4—Sr1 ⁱⁱⁱ | 46.00 (14) |
| O14—Sr3—O3 ^{viii} | 95.10 (13) | O3 ^{xvi} —As4—Sr1 ⁱⁱⁱ | 124.19 (13) |
| O8 ^{vii} —Sr3—O3 ^{viii} | 80.40 (12) | O4—As4—Sr1 ⁱⁱⁱ | 54.37 (12) |
| O13 ⁱⁱ —Sr3—O3 ^{viii} | 74.08 (12) | Sr4 ^{xvi} —As4—Sr1 ⁱⁱⁱ | 97.122 (16) |
| O10 ⁱⁱ —Sr3—O7 ⁱⁱ | 73.13 (13) | O1 ^{xv} —As4—Sr3 ^{xvii} | 34.11 (13) |
| O1 ^{vii} —Sr3—O7 ⁱⁱ | 75.77 (13) | O2—As4—Sr3 ^{xvii} | 89.22 (14) |
| O14—Sr3—O7 ⁱⁱ | 140.63 (13) | O3 ^{xvi} —As4—Sr3 ^{xvii} | 109.59 (13) |
| O8 ^{vii} —Sr3—O7 ⁱⁱ | 116.38 (12) | O4—As4—Sr3 ^{xvii} | 134.84 (13) |
| O13 ⁱⁱ —Sr3—O7 ⁱⁱ | 59.20 (11) | Sr4 ^{xvi} —As4—Sr3 ^{xvii} | 92.470 (16) |
| O3 ^{viii} —Sr3—O7 ⁱⁱ | 118.18 (12) | Sr1 ⁱⁱⁱ —As4—Sr3 ^{xvii} | 116.588 (18) |
| O10 ⁱⁱ —Sr3—O12 | 55.50 (11) | O1 ^{xv} —As4—Sr4 ^{xv} | 33.42 (13) |
| O1 ^{vii} —Sr3—O12 | 84.94 (11) | O2—As4—Sr4 ^{xv} | 124.04 (14) |
| O14—Sr3—O12 | 75.56 (12) | O3 ^{xvi} —As4—Sr4 ^{xv} | 126.42 (13) |
| O8 ^{vii} —Sr3—O12 | 158.38 (11) | O4—As4—Sr4 ^{xv} | 73.99 (13) |
| O13 ⁱⁱ —Sr3—O12 | 125.74 (11) | Sr4 ^{xvi} —As4—Sr4 ^{xv} | 155.21 (2) |
| O3 ^{viii} —Sr3—O12 | 114.35 (11) | Sr1 ⁱⁱⁱ —As4—Sr4 ^{xv} | 101.419 (16) |
| O7 ⁱⁱ —Sr3—O12 | 71.92 (11) | Sr3 ^{xvii} —As4—Sr4 ^{xv} | 64.541 (13) |
| O10 ⁱⁱ —Sr3—As1 ⁱⁱ | 80.01 (10) | O1 ^{xv} —As4—Sr3 ^{xviii} | 135.30 (14) |
| O1 ^{vii} —Sr3—As1 ⁱⁱ | 88.50 (9) | O2—As4—Sr3 ^{xviii} | 105.79 (14) |

| | | | |
|---|--------------|---|--------------|
| O14—Sr3—As1 ⁱⁱ | 167.75 (10) | O3 ^{xvi} —As4—Sr3 ^{xviii} | 37.06 (13) |
| O8 ^{vii} —Sr3—As1 ⁱⁱ | 93.63 (9) | O4—As4—Sr3 ^{xviii} | 73.24 (13) |
| O13 ⁱⁱ —Sr3—As1 ⁱⁱ | 29.41 (8) | Sr4 ^{xvi} —As4—Sr3 ^{xviii} | 70.193 (14) |
| O3 ^{viii} —Sr3—As1 ⁱⁱ | 97.14 (8) | Sr1 ⁱⁱⁱ —As4—Sr3 ^{xviii} | 94.890 (16) |
| O7 ⁱⁱ —Sr3—As1 ⁱⁱ | 29.83 (8) | Sr3 ^{xvii} —As4—Sr3 ^{xviii} | 146.09 (2) |
| O12—Sr3—As1 ⁱⁱ | 99.72 (7) | Sr4 ^{xv} —As4—Sr3 ^{xviii} | 123.790 (16) |
| O10 ⁱⁱ —Sr3—As2 | 27.08 (9) | O1 ^{xv} —As4—Sr1 ^{xix} | 80.74 (14) |
| O1 ^{vii} —Sr3—As2 | 110.07 (8) | O2—As4—Sr1 ^{xix} | 127.56 (14) |
| O14—Sr3—As2 | 93.94 (9) | O3 ^{xvi} —As4—Sr1 ^{xix} | 32.57 (13) |
| O8 ^{vii} —Sr3—As2 | 171.48 (9) | O4—As4—Sr1 ^{xix} | 121.76 (12) |
| O13 ⁱⁱ —Sr3—As2 | 104.64 (8) | Sr4 ^{xvi} —As4—Sr1 ^{xix} | 67.769 (14) |
| O3 ^{viii} —Sr3—As2 | 91.14 (8) | Sr1 ⁱⁱⁱ —As4—Sr1 ^{xix} | 156.76 (2) |
| O7 ⁱⁱ —Sr3—As2 | 66.78 (8) | Sr3 ^{xvii} —As4—Sr1 ^{xix} | 82.756 (15) |
| O12—Sr3—As2 | 28.80 (7) | Sr4 ^{xv} —As4—Sr1 ^{xix} | 98.608 (16) |
| As1 ⁱⁱ —Sr3—As2 | 86.359 (17) | Sr3 ^{xviii} —As4—Sr1 ^{xix} | 63.894 (13) |
| O10 ⁱⁱ —Sr3—As4 ^{ix} | 116.55 (9) | As4 ^{xx} —O1—Sr3 ^{xxi} | 123.83 (18) |
| O1 ^{vii} —Sr3—As4 ^{ix} | 22.06 (8) | As4 ^{xx} —O1—Sr4 | 125.37 (19) |
| O14—Sr3—As4 ^{ix} | 71.77 (10) | Sr3 ^{xxi} —O1—Sr4 | 104.52 (13) |
| O8 ^{vii} —Sr3—As4 ^{ix} | 98.65 (9) | As4—O2—Sr1 ⁱⁱⁱ | 106.54 (17) |
| O13 ⁱⁱ —Sr3—As4 ^{ix} | 118.28 (8) | As4—O2—Sr2 ^{xxii} | 142.5 (2) |
| O3 ^{viii} —Sr3—As4 ^{ix} | 166.86 (8) | Sr1 ⁱⁱⁱ —O2—Sr2 ^{xxii} | 100.24 (13) |
| O7 ⁱⁱ —Sr3—As4 ^{ix} | 74.11 (8) | As4—O2—Sr4 ^{xvi} | 89.82 (15) |
| O12—Sr3—As4 ^{ix} | 63.25 (7) | Sr1 ⁱⁱⁱ —O2—Sr4 ^{xvi} | 134.85 (15) |
| As1 ⁱⁱ —Sr3—As4 ^{ix} | 95.994 (17) | Sr2 ^{xxii} —O2—Sr4 ^{xvi} | 89.51 (10) |
| As2—Sr3—As4 ^{ix} | 89.820 (16) | As4 ^{xiii} —O3—Sr1 ⁱⁱⁱ | 126.87 (19) |
| O10 ⁱⁱ —Sr3—As3 ^{viii} | 133.38 (9) | As4 ^{xiii} —O3—Sr3 ^{xii} | 120.60 (19) |
| O1 ^{vii} —Sr3—As3 ^{viii} | 90.92 (9) | Sr1 ⁱⁱⁱ —O3—Sr3 ^{xii} | 100.82 (13) |
| O14—Sr3—As3 ^{viii} | 73.01 (9) | As4 ^{xiii} —O3—Sr4 | 100.96 (17) |
| O8 ^{vii} —Sr3—As3 ^{viii} | 21.27 (9) | Sr1 ⁱⁱⁱ —O3—Sr4 | 100.88 (12) |
| O13 ⁱⁱ —Sr3—As3 ^{viii} | 85.58 (8) | Sr3 ^{xii} —O3—Sr4 | 102.36 (12) |
| O3 ^{viii} —Sr3—As3 ^{viii} | 67.59 (8) | As4—O4—As3 ^{xvi} | 126.8 (2) |
| O7 ⁱⁱ —Sr3—As3 ^{viii} | 137.00 (8) | As4—O4—Sr1 ⁱⁱⁱ | 95.02 (14) |
| O12—Sr3—As3 ^{viii} | 148.54 (7) | As3 ^{xvi} —O4—Sr1 ⁱⁱⁱ | 137.87 (18) |
| As1 ⁱⁱ —Sr3—As3 ^{viii} | 111.362 (17) | As3—O5—Sr1 | 116.2 (2) |
| As2—Sr3—As3 ^{viii} | 153.25 (2) | As3—O5—Sr4 ⁱⁱ | 122.23 (19) |
| As4 ^{ix} —Sr3—As3 ^{viii} | 107.264 (16) | Sr1—O5—Sr4 ⁱⁱ | 102.39 (13) |
| O1—Sr4—O10 ^x | 110.84 (12) | As3—O5—Sr2 ⁱⁱⁱ | 90.31 (16) |
| O1—Sr4—O12 ^{xi} | 83.45 (13) | Sr1—O5—Sr2 ⁱⁱⁱ | 93.78 (12) |
| O10 ^x —Sr4—O12 ^{xi} | 152.75 (13) | Sr4 ⁱⁱ —O5—Sr2 ⁱⁱⁱ | 129.62 (15) |
| O1—Sr4—O8 | 75.33 (12) | As1—O6—As2 | 129.3 (2) |
| O10 ^x —Sr4—O8 | 132.54 (13) | As1—O6—Sr4 ^{viii} | 133.0 (2) |
| O12 ^{xi} —Sr4—O8 | 72.49 (13) | As2—O6—Sr4 ^{viii} | 94.63 (15) |
| O1—Sr4—O5 ⁱⁱⁱ | 82.29 (12) | As1—O7—Sr1 ⁱⁱ | 115.01 (19) |
| O10 ^x —Sr4—O5 ⁱⁱⁱ | 70.56 (14) | As1—O7—Sr2 | 94.57 (18) |
| O12 ^{xi} —Sr4—O5 ⁱⁱⁱ | 89.41 (13) | Sr1 ⁱⁱ —O7—Sr2 | 97.04 (13) |
| O8—Sr4—O5 ⁱⁱⁱ | 152.48 (13) | As1—O7—Sr3 ⁱⁱⁱ | 90.74 (16) |
| O1—Sr4—O3 | 158.86 (13) | Sr1 ⁱⁱ —O7—Sr3 ⁱⁱⁱ | 127.25 (16) |
| O10 ^x —Sr4—O3 | 64.49 (11) | Sr2—O7—Sr3 ⁱⁱⁱ | 127.44 (15) |

| | | | |
|--|-------------|---|-------------|
| O12 ^{xi} —Sr4—O3 | 93.63 (12) | As3 ⁱ —O8—Sr3 ^{xxi} | 126.29 (19) |
| O8—Sr4—O3 | 123.82 (11) | As3 ⁱ —O8—Sr4 | 107.61 (17) |
| O5 ⁱⁱⁱ —Sr4—O3 | 76.73 (11) | Sr3 ^{xxi} —O8—Sr4 | 101.60 (13) |
| O1—Sr4—O6 ^{xii} | 68.82 (11) | As3 ⁱ —O8—Sr2 ^{xxiii} | 103.66 (17) |
| O10 ^x —Sr4—O6 ^{xii} | 56.58 (11) | Sr3 ^{xxi} —O8—Sr2 ^{xxiii} | 114.81 (14) |
| O12 ^{xi} —Sr4—O6 ^{xii} | 148.69 (12) | Sr4—O8—Sr2 ^{xxiii} | 99.49 (12) |
| O8—Sr4—O6 ^{xii} | 86.22 (11) | As2 ⁱⁱⁱ —O9—Sr1 | 119.1 (2) |
| O5 ⁱⁱⁱ —Sr4—O6 ^{xii} | 100.56 (11) | As2 ⁱⁱⁱ —O9—Sr2 | 120.05 (18) |
| O3—Sr4—O6 ^{xii} | 117.48 (11) | Sr1—O9—Sr2 | 113.29 (14) |
| O1—Sr4—O2 ^{xiii} | 136.97 (11) | As2 ⁱⁱⁱ —O10—Sr3 ⁱⁱⁱ | 110.6 (2) |
| O10 ^x —Sr4—O2 ^{xiii} | 110.59 (11) | As2 ⁱⁱⁱ —O10—Sr4 ^{xxiv} | 110.98 (18) |
| O12 ^{xi} —Sr4—O2 ^{xiii} | 64.36 (11) | Sr3 ⁱⁱⁱ —O10—Sr4 ^{xxiv} | 111.31 (15) |
| O8—Sr4—O2 ^{xiii} | 68.43 (11) | As3—O11—Sr2 ⁱ | 142.2 (2) |
| O5 ⁱⁱⁱ —Sr4—O2 ^{xiii} | 122.63 (11) | As3—O11—Sr4 ^{iv} | 85.43 (17) |
| O3—Sr4—O2 ^{xiii} | 56.92 (10) | Sr2 ⁱ —O11—Sr4 ^{iv} | 128.41 (16) |
| O6 ^{xii} —Sr4—O2 ^{xiii} | 128.82 (11) | As2—O12—Sr2 ^{iv} | 125.5 (2) |
| O1—Sr4—O11 ⁱ | 108.85 (12) | As2—O12—Sr4 ^{xiv} | 126.0 (2) |
| O10 ^x —Sr4—O11 ⁱ | 80.77 (12) | Sr2 ^{iv} —O12—Sr4 ^{xiv} | 101.82 (14) |
| O12 ^{xi} —Sr4—O11 ⁱ | 117.54 (11) | As2—O12—Sr3 | 82.01 (16) |
| O8—Sr4—O11 ⁱ | 54.27 (11) | Sr2 ^{iv} —O12—Sr3 | 94.25 (13) |
| O5 ⁱⁱⁱ —Sr4—O11 ⁱ | 151.33 (12) | Sr4 ^{xiv} —O12—Sr3 | 122.43 (15) |
| O3—Sr4—O11 ⁱ | 91.11 (11) | As1—O13—Sr1 ^{iv} | 116.89 (19) |
| O6 ^{xii} —Sr4—O11 ⁱ | 61.93 (11) | As1—O13—Sr3 ⁱⁱⁱ | 100.95 (16) |
| O2 ^{xiii} —Sr4—O11 ⁱ | 67.23 (11) | Sr1 ^{iv} —O13—Sr3 ⁱⁱⁱ | 102.21 (13) |
| O1—Sr4—As4 ^{xiii} | 156.53 (9) | As1—O13—Sr2 ^{iv} | 124.42 (18) |
| O10 ^x —Sr4—As4 ^{xiii} | 90.53 (8) | Sr1 ^{iv} —O13—Sr2 ^{iv} | 103.48 (12) |
| O12 ^{xi} —Sr4—As4 ^{xiii} | 73.09 (9) | Sr3 ⁱⁱⁱ —O13—Sr2 ^{iv} | 106.22 (13) |
| O8—Sr4—As4 ^{xiii} | 97.70 (8) | As1 ^{iv} —O14—Sr3 | 143.5 (2) |
| O5 ⁱⁱⁱ —Sr4—As4 ^{xiii} | 96.52 (8) | As1 ^{iv} —O14—Sr2 ^{iv} | 95.30 (18) |
| O3—Sr4—As4 ^{xiii} | 28.72 (8) | Sr3—O14—Sr2 ^{iv} | 107.87 (14) |
| O6 ^{xii} —Sr4—As4 ^{xiii} | 133.87 (8) | | |

Symmetry codes: (i) $-y, x, z-1/4$; (ii) $y, -x+1, z+1/4$; (iii) $-y+1, x, z-1/4$; (iv) $y, -x, z+1/4$; (v) $-x, -y+1, z+1/2$; (vi) $-x+1, -y+1, z+1/2$; (vii) $x, y, z+1$; (viii) $-y, x, z+3/4$; (ix) $-y+1, x-1, z+3/4$; (x) $-x+1, -y, z-1/2$; (xi) $y, -x+1, z-3/4$; (xii) $y, -x, z-3/4$; (xiii) $x-1, y, z$; (xiv) $-y+1, x, z+3/4$; (xv) $y+1, -x+1, z+1/4$; (xvi) $x+1, y, z$; (xvii) $y+1, -x+1, z-3/4$; (xviii) $y+1, -x, z-3/4$; (xix) $-y+2, x, z-1/4$; (xx) $-y+1, x-1, z-1/4$; (xxi) $x, y, z-1$; (xxii) $-x+1, -y+1, z-1/2$; (xxiii) $-x, -y+1, z-1/2$; (xxiv) $-x+1, -y, z+1/2$.