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 The aluminioarsenate $K_{1.8}Sr_{0.6}Al_3(AsO_4)_4$

 Anissa Haj Abdallah^{a*} and Amor Haddad^b

^aInstitut Supérieur des Sciences Appliquées et Technologie de Gabès, Avenue Omar Ibn El Khatlab, 6072 Zrig, Gabès, Tunisia, and ^bLaboratoire de Matériaux et Cristalochimie, Institut Supérieur des Sciences Appliquées et Technologie de Mahdia, Avenue El Mourouj, Sidi Messoud 5111 Hiboun, Mahdia, Tunisia
Correspondence e-mail: haj_anissa@yahoo.fr

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(Al-O) = 0.004$ Å; disorder in main residue; R factor = 0.039; wR factor = 0.112; data-to-parameter ratio = 9.0.

The title compound, potassium strontium trialuminium tetraarsenate, was prepared by solid-state reaction. The structure consists of AlO_6 octahedra (site symmetries $2..$ and $2/m$) and two AsO_4 tetrahedra ($.2.$ and $m..$) sharing corners and edges to form a two-dimensional structure parallel to (010). The cations are occupationally disordered and are located in the interlayer space. For both types of cations, distorted coordination polyhedra are observed.

Related literature

For further information on this structure type, see: $K_3Cr_3(AsO_4)_4$ (Friaa *et al.*, 2003); $K_3Fe_3(AsO_4)_4$ (Ouerfelli *et al.*, 2005). For similar structures, see: $K_3Fe_3(PO_4)_4 \cdot H_2O$ (Lii, 1995); $Na_3Fe_3(PO_4)_4$ (Lajmi *et al.*, 2002). For background to the bond-valence method, see: Brown & Altermatt (1985).

Experimental

Crystal data

 $K_{1.8}Sr_{0.6}Al_3(AsO_4)_4$
 $M_r = 759.57$

 Orthorhombic, $Cmce$
 $a = 10.567$ (3) Å

 $b = 20.531$ (4) Å
 $c = 6.388$ (1) Å
 $V = 1385.9$ (5) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 12.67$ mm⁻¹
 $T = 293$ K
 $0.36 \times 0.22 \times 0.14$ mm

Data collection

 Enraf–Nonius CAD-4
 diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{min} = 0.088$, $T_{max} = 0.292$
 1510 measured reflections

 796 independent reflections
 704 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.024$
 2 standard reflections every 120 min
 intensity decay: 0.4%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.112$
 $S = 1.09$
 796 reflections

 88 parameters
 $\Delta\rho_{max} = 1.68$ e Å⁻³
 $\Delta\rho_{min} = -1.45$ e Å⁻³

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2195).

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supporting information

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The aluminoarsenate $K_{1.8}Sr_{0.6}Al_3(AsO_4)_4$

Anissa Haj Abdallah and Amor Haddad

S1. Comment

The crystal structure of $K_{1.8}Sr_{0.6}Al_3(AsO_4)_4$ is a two-dimensional network formed by curved layers perpendicular to the b axis. Each layer consists of AlO_6 octahedra and AsO_4 tetrahedra sharing corners and edges (Fig. 1). This structural arrangement leads to six-membered windows within the layer (Fig. 2). It is isostructural with the compounds $K_3Cr_3(AsO_4)_4$ (Friaa *et al.*, 2003) and $K_3Fe_3(AsO_4)_4$ (Ouerfelli *et al.*, 2005). The asymmetric unit is the link-up of two AlO_6 octahedra and As_2O_4 tetrahedron by corners and As_1O_4 tetrahedron by edges (Fig. 3). The common edge $O4 \cdots O4$, is the shortest oxygen distance. The As_1O_4 tetrahedron lies on two fold axis and is distorted. It has two type of $As-O$ bonds, two short distances and two long distances involving the bridging oxygen atoms $O4$. The As_2O_4 tetrahedron is located on mirror plane. It shares two oxygen atoms $O5$ with two equivalent Al_1O_6 octahedra and one oxygen atom $O1$, which is situated on mirror plane, with Al_2O_6 octahedron. The fourth oxygen atom $O2$ which lies on mirror plane is not coordinated and points to the interlayer space. The Al_1O_6 octahedron is strongly distorted which the $O4-Al_1-O4$ angle 75.6° is more acute than those according to an ideal octahedron. The mean distance of Al_1-O 1.930 (4) Å. The Al_2O_6 octahedron which lies on a crystallographic center of symmetry is less distorted than the Al_1O_6 octahedron which lies on a two fold axis. The structure is characterized by two cationic sites. The site (0, 1/2, 1/2) located in the interlayer space and the site (1/4, 1/2, 1/4) confined in windows. The difference to be indicated is the cationic distribution in the similar structure compounds. Both strontium cations $Sr1$ and $Sr2$ occupy the windows and the potassium cations $K1$ and $K2$ are located in interlayers space of the structure. The bond valence sum of the $K1$, $K2$ and $Sr1$ are in a good agreement with their oxidation states (Brown & Altermatt, 1985). But for the $Sr2$, the bond strength is higher than the expected value +2 suggesting that the SrO_6 appear too small for this ion which is acceptable given the small number of Sr atoms that occupy this site. The valence sums around the Al atoms are both low (2.6 vu) but attempts to introduce other elements onto these sites were not successful. The resulting difference electron density contains several large features reflecting the difficulty in determining the precise locations of Sr and K .

S2. Experimental

The purpose is to obtain a phase from the molars proportions of (2:0.5:4) of a mixture of KNO_3 , $Sr(NO_3)_2$ and $NH_4H_2AsO_4$. The mixture was finely ground and calcined at 723 K in a porcelain crucible. Then the temperature was held at 943 K during 26 h. A slow cooling in a speed of 2 K/h until 893 K and of 5 K/h until 823 K was proceeded. The fusion was reached. A long wash in the boiling water allowed us to isolate some parallelepipedic colourless crystals with acceptable size for an analysis by X-ray diffraction on single-crystal. The qualitative analysis by electron microscope probe of a selected crystal revealed the presence of aluminium atom which comes from the crucible, as well as the different elements of the compound composition.

S3. Refinement

The localization of the strontium and potassium atoms is delicate because of the existence of disorder. The Fourier difference synthesis reveals an intense peak and three nearby peaks relatively less intense. It was then necessary to take considering the peaks which could have a structural meaning because of their environments in atoms of oxygen. A constraint, respecting the electroneutrality, was applied to the occupation rates of the cations. Furthermore, the refinement anisotropy leading to very deformed ellipsoids, the condition EADP allowed by the program SHELX was applied. The high value of the electron densities occurs at $1.68 \text{ e}/\text{A}^3$ from heavy atom As1 is due to the effects of Fourier series termination.

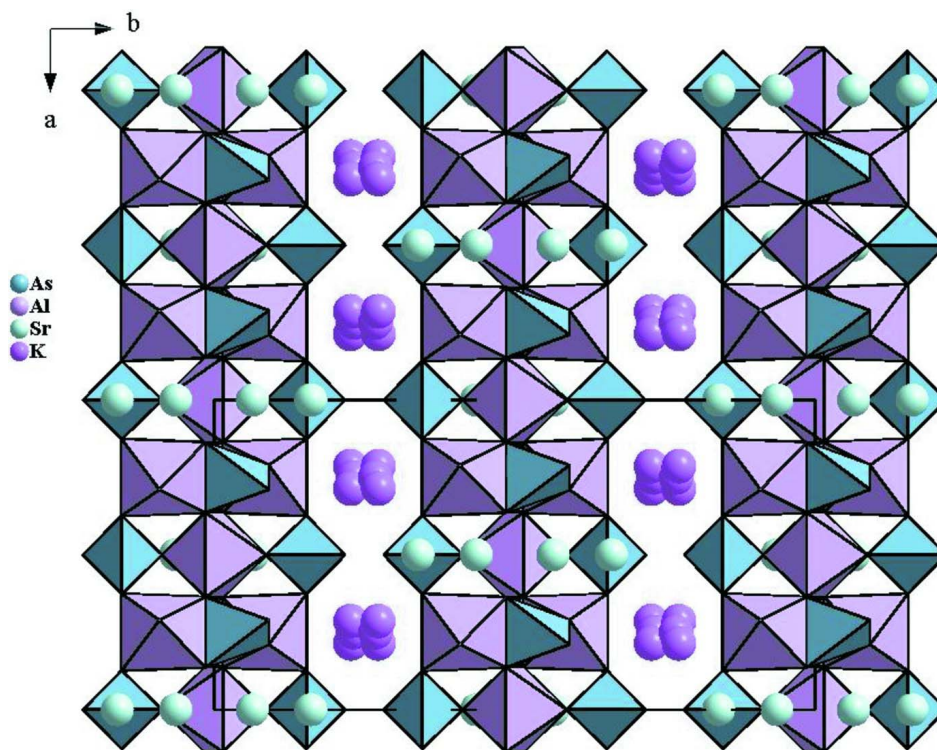


Figure 1

Projection of the structure of $\text{K}_{1.8}\text{Sr}_{0.6}\text{Al}_3(\text{AsO}_4)_4$ along the c axis.

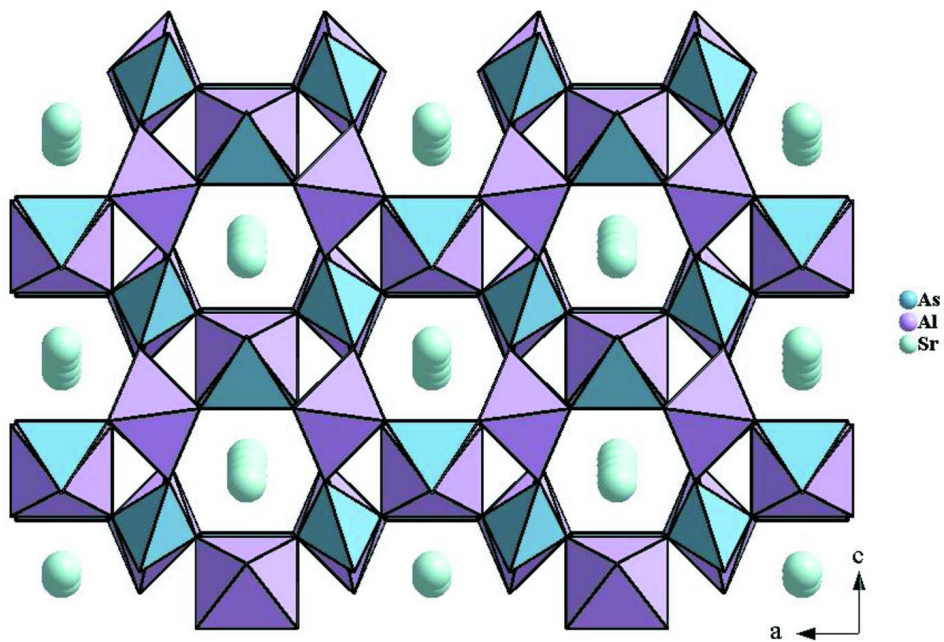


Figure 2

A view of a layer showing the windows.

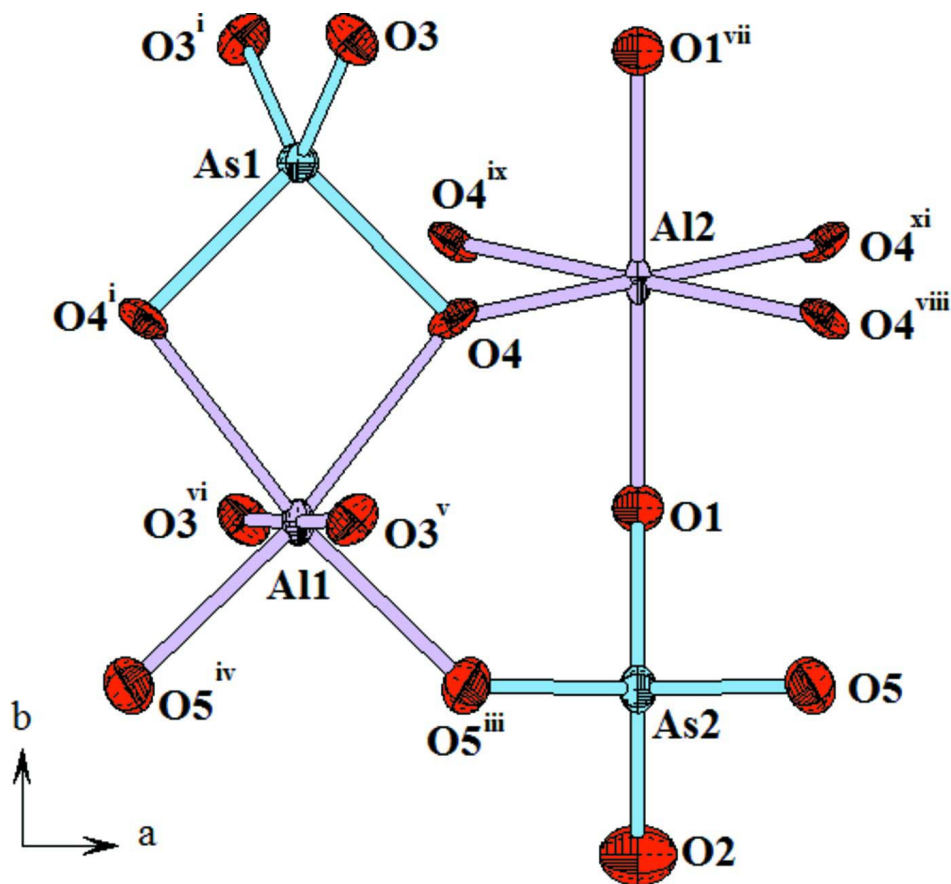


Figure 3

The asymmetric unit of the structure of $\text{K}_{1.8}\text{Sr}_{0.6}\text{Al}_3(\text{AsO}_4)_4$.

potassium strontium trialuminium tetraarsenate

Crystal data

$\text{K}_{1.8}\text{Sr}_{0.6}\text{Al}_3(\text{AsO}_4)_4$

$M_r = 759.57$

Orthorhombic, $Cmce$

Hall symbol: $-C\ 2bc\ 2$

$a = 10.567\ (3)\ \text{\AA}$

$b = 20.531\ (4)\ \text{\AA}$

$c = 6.388\ (1)\ \text{\AA}$

$V = 1385.9\ (5)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1424$

$D_x = 3.641\ \text{Mg m}^{-3}$

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

Cell parameters from 25 reflections

$\theta = 2.2\text{--}27^\circ$

$\mu = 12.67\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Parallelepiped, colourless

$0.36 \times 0.22 \times 0.14\ \text{mm}$

Data collection

Enraf–Nonius CAD-4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

$T_{\min} = 0.088$, $T_{\max} = 0.292$

1510 measured reflections

796 independent reflections

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

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 3.8^\circ$

$h = -13 \rightarrow 0$

$k = -26 \rightarrow 0$

$l = -8 \rightarrow 8$

2 standard reflections every 120 min

intensity decay: 0.4%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.112$

$S = 1.09$

796 reflections

88 parameters

0 restraints

Primary atom site location: real-space vector search

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.68 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.45 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0006 (3)

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	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
As1	0.7500	0.54444 (4)	0.2500	0.0058 (3)	
As2	0.0000	0.65488 (4)	-0.05958 (11)	0.0070 (3)	
Al1	0.7500	0.40809 (11)	0.2500	0.0054 (5)	
Al2	0.0000	0.5000	0.0000	0.0069 (6)	
Sr1	0.010 (3)	0.6619 (4)	0.4463 (8)	0.056 (4)	0.12 (2)
Sr2	0.006 (8)	0.5644 (17)	0.477 (4)	0.056 (4)	0.03 (2)
K1	0.2111 (8)	0.7265 (4)	0.3993 (12)	0.062 (2)	0.33 (1)
K2	0.258 (2)	0.7305 (10)	0.190 (3)	0.062 (2)	0.12 (1)
O1	0.0000	0.5866 (3)	0.0858 (7)	0.0090 (10)	
O2	0.0000	0.7176 (3)	0.1009 (9)	0.0180 (12)	
O3	0.7104 (3)	0.59095 (18)	0.0477 (5)	0.0092 (7)	
O4	0.6367 (3)	0.48557 (16)	0.2962 (5)	0.0078 (7)	
O5	-0.1259 (3)	0.65351 (18)	-0.2222 (5)	0.0120 (8)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.0061 (4)	0.0055 (4)	0.0057 (4)	0.000	0.0008 (2)	0.000
As2	0.0047 (4)	0.0081 (4)	0.0083 (4)	0.000	0.000	-0.0014 (2)
Al1	0.0042 (10)	0.0075 (11)	0.0046 (9)	0.000	0.0008 (6)	0.000
Al2	0.0026 (13)	0.0090 (15)	0.0088 (13)	0.000	0.000	0.0000 (11)
Sr1	0.058 (7)	0.074 (5)	0.034 (2)	0.038 (9)	-0.004 (5)	0.003 (2)
Sr2	0.058 (7)	0.074 (5)	0.034 (2)	0.038 (9)	-0.004 (5)	0.003 (2)
K1	0.074 (5)	0.051 (3)	0.060 (5)	0.037 (4)	-0.002 (4)	0.011 (3)
K2	0.074 (5)	0.051 (3)	0.060 (5)	0.037 (4)	-0.002 (4)	0.011 (3)

O1	0.008 (2)	0.008 (2)	0.010 (2)	0.000	0.000	0.0038 (19)
O2	0.022 (3)	0.014 (3)	0.018 (3)	0.000	0.000	-0.004 (2)
O3	0.0094 (17)	0.0098 (18)	0.0084 (15)	0.0029 (15)	-0.0011 (13)	0.0003 (13)
O4	0.0086 (16)	0.0060 (16)	0.0088 (15)	-0.0033 (15)	0.0017 (14)	0.0011 (11)
O5	0.0089 (18)	0.0115 (17)	0.0155 (18)	-0.0023 (16)	-0.0024 (14)	0.0051 (13)

Geometric parameters (Å, °)

As1—O3 ⁱ	1.661 (3)	Sr1—O2	2.489 (8)
As1—O3	1.661 (3)	Sr1—O5 ^{xiii}	2.565 (17)
As1—O4 ⁱ	1.727 (3)	Sr1—O3 ^{ix}	2.57 (2)
As1—O4	1.727 (3)	Sr1—O2 ^{xiv}	2.666 (10)
As2—O2	1.646 (6)	Sr1—O3 ^{xi}	2.75 (3)
As2—O1	1.682 (5)	Sr1—O1	2.775 (9)
As2—O5 ⁱⁱ	1.688 (3)	Sr2—O3 ^{ix}	2.23 (9)
As2—O5	1.688 (3)	Sr2—O4 ^{xv}	2.67 (4)
Al1—O5 ⁱⁱⁱ	1.831 (4)	Sr2—O4 ^{ix}	2.75 (4)
Al1—O5 ^{iv}	1.831 (4)	Sr2—O1	2.54 (2)
Al1—O3 ^v	1.947 (3)	Sr2—O5 ^{xii}	2.94 (5)
Al1—O3 ^{vi}	1.947 (3)	Sr2—O3 ^{xi}	2.36 (8)
Al1—O4 ⁱ	2.013 (4)	K1—O5 ^{xiv}	2.735 (7)
Al1—O4	2.013 (4)	K1—O3 ^{ix}	2.804 (8)
Al2—O1 ^{vii}	1.861 (5)	K1—O2 ^{xiv}	2.819 (8)
Al2—O1	1.861 (5)	K1—O2	2.940 (9)
Al2—O4 ^{viii}	1.967 (3)	K2—O5 ^{xvi}	2.69 (2)
Al2—O4 ^{ix}	1.967 (3)	K2—O2	2.80 (3)
Al2—O4 ^x	1.967 (3)	K2—O5 ^{xiv}	2.817 (19)
Al2—O4 ^{xi}	1.967 (3)	K2—O2 ^{xvii}	2.90 (2)
Sr1—O5 ^{xii}	2.450 (15)	K2—O3 ^{xviii}	3.02 (2)
O3 ⁱ —As1—O3	109.8 (2)	O5 ^{xiii} —Sr1—O3 ^{ix}	114.3 (3)
O3 ⁱ —As1—O4 ⁱ	111.16 (17)	O5 ^{xii} —Sr1—O2 ^{xiv}	76.4 (3)
O3—As1—O4 ⁱ	116.37 (16)	O2—Sr1—O2 ^{xiv}	84.2 (2)
O3 ⁱ —As1—O4	116.37 (16)	O5 ^{xiii} —Sr1—O2 ^{xiv}	74.6 (3)
O3—As1—O4	111.16 (17)	O3 ^{ix} —Sr1—O2 ^{xiv}	123.7 (9)
O4 ⁱ —As1—O4	91.2 (2)	O5 ^{xii} —Sr1—O3 ^{xi}	112.0 (5)
O2—As2—O1	108.0 (3)	O2—Sr1—O3 ^{xi}	102.6 (7)
O2—As2—O5 ⁱⁱ	113.34 (17)	O5 ^{xiii} —Sr1—O3 ^{xi}	58.5 (5)
O1—As2—O5 ⁱⁱ	109.03 (16)	O3 ^{ix} —Sr1—O3 ^{xi}	113.5 (3)
O2—As2—O5	113.34 (17)	O2 ^{xiv} —Sr1—O3 ^{xi}	116.9 (8)
O1—As2—O5	109.03 (16)	O5 ^{xii} —Sr1—O1	134.2 (6)
O5 ⁱⁱ —As2—O5	104.0 (2)	O2—Sr1—O1	61.2 (2)
O5 ⁱⁱⁱ —Al1—O5 ^{iv}	92.6 (2)	O5 ^{xiii} —Sr1—O1	128.7 (9)
O5 ⁱⁱⁱ —Al1—O3 ^v	93.80 (16)	O3 ^{ix} —Sr1—O1	74.3 (3)
O5 ^{iv} —Al1—O3 ^v	87.00 (16)	O2 ^{xiv} —Sr1—O1	145.3 (3)
O5 ⁱⁱⁱ —Al1—O3 ^{vi}	87.00 (16)	O3 ^{xi} —Sr1—O1	71.6 (4)
O5 ^{iv} —Al1—O3 ^{vi}	93.80 (16)	O3 ^{ix} —Sr2—O4 ^{xv}	69 (2)
O3 ^v —Al1—O3 ^{vi}	178.8 (3)	O3 ^{ix} —Sr2—O4 ^{ix}	67.4 (18)

O5 ⁱⁱⁱ —A11—O4 ⁱ	96.06 (14)	O4 ^{xv} —Sr2—O4 ^{ix}	90.0 (17)
O5 ^{iv} —A11—O4 ⁱ	170.55 (17)	O3 ^{ix} —Sr2—O1	85.0 (19)
O3 ^v —A11—O4 ⁱ	88.66 (15)	O4 ^{xv} —Sr2—O1	147 (3)
O3 ^{vi} —A11—O4 ⁱ	90.43 (15)	O4 ^{ix} —Sr2—O1	59.7 (7)
O5 ⁱⁱⁱ —A11—O4	170.55 (17)	O4 ^{xv} —Sr2—O5 ^{xii}	61.2 (11)
O5 ^{iv} —A11—O4	96.06 (14)	O4 ^{ix} —Sr2—O5 ^{xii}	125 (3)
O3 ^v —A11—O4	90.43 (15)	O1—Sr2—O5 ^{xii}	123 (2)
O3 ^{vi} —A11—O4	88.66 (15)	O3 ^{ix} —Sr2—O3 ^{xi}	151.3 (17)
O4 ⁱ —A11—O4	75.6 (2)	O4 ^{xv} —Sr2—O3 ^{xi}	130 (2)
O1 ^{vii} —A12—O1	180.0 (3)	O4 ^{ix} —Sr2—O3 ^{xi}	125 (2)
O1 ^{vii} —A12—O4 ^{viii}	87.08 (14)	O1—Sr2—O3 ^{xi}	82.4 (17)
O1—A12—O4 ^{viii}	92.92 (14)	O5 ^{xii} —Sr2—O3 ^{xi}	108.5 (13)
O1 ^{vii} —A12—O4 ^{ix}	92.92 (14)	O5 ^{xiv} —K1—O3 ^{ix}	158.0 (4)
O1—A12—O4 ^{ix}	87.08 (14)	O5 ^{xiv} —K1—O2 ^{xiv}	60.2 (2)
O4 ^{viii} —A12—O4 ^{ix}	85.5 (2)	O3 ^{ix} —K1—O2 ^{xiv}	110.3 (3)
O1 ^{vii} —A12—O4 ^x	87.08 (14)	O5 ^{xiv} —K1—O2	67.8 (2)
O1—A12—O4 ^x	92.92 (14)	O3 ^{ix} —K1—O2	90.8 (3)
O4 ^{viii} —A12—O4 ^x	94.5 (2)	O2 ^{xiv} —K1—O2	73.8 (2)
O4 ^{ix} —A12—O4 ^x	180.0	O5 ^{xvi} —K2—O2	123.0 (7)
O1 ^{vii} —A12—O4 ^{xii}	92.92 (14)	O5 ^{xvi} —K2—O5 ^{xiv}	57.4 (4)
O1—A12—O4 ^{xii}	87.08 (14)	O2—K2—O5 ^{xiv}	68.8 (5)
O4 ^{viii} —A12—O4 ^{xii}	180.00 (19)	O5 ^{xvi} —K2—O2 ^{xvii}	69.0 (6)
O4 ^{ix} —A12—O4 ^{xii}	94.5 (2)	O2—K2—O2 ^{xvii}	160.9 (8)
O4 ^x —A12—O4 ^{xii}	85.5 (2)	O5 ^{xiv} —K2—O2 ^{xvii}	114.9 (8)
O5 ^{xii} —Sr1—O2	145.1 (10)	O5 ^{xvi} —K2—O3 ^{xviii}	144.3 (9)
O5 ^{xii} —Sr1—O5 ^{xiii}	64.0 (2)	O2—K2—O3 ^{xviii}	87.6 (7)
O2—Sr1—O5 ^{xiii}	137.6 (9)	O5 ^{xiv} —K2—O3 ^{xviii}	156.4 (10)
O5 ^{xii} —Sr1—O3 ^{ix}	62.4 (5)	O2 ^{xvii} —K2—O3 ^{xviii}	87.4 (5)
O2—Sr1—O3 ^{ix}	108.1 (7)		

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