inorganic compounds

The aluminoarsenate Na$_{1.67}$K$_{1.33}$Al$_3$(AsO$_4$)$_4$

Mohamad Alem Bouhassine and Habib Boughzala*

Laboratoire des Materiaux et de Cristallochimie, Faculte des Sciences de Tunis, Tunisia
Correspondence e-mail: habib.boughzala@ipein.rnu.tn

The title compound, sodium potassium trialuminium tetrakis(orthoarsenate), was prepared by solid-state reactions. The anionic framework consists of corrugated layers parallel to (010) and is made up of corner-sharing AlO$_6$ octahedra (site symmetries .2. and 2/m..) that are connected to isolated AsO$_4$ tetrahedra (site symmetries .2. and m..) through edge- and corner-sharing. The alkali cations are occupationally disordered. The two K$^+$ cations [site symmetries .2. and m..; occupancies 0.314 (7) and 0.035 (12)] are situated in the interlayer space, whereas the smaller Na$^+$ cations [both with site symmetry m..; occupancies = 0.725 (14) and 0.112 (14)] are located in the cavities of the anionic framework. The K$^+$ cations are surrounded by six and seven O atoms, the Na$^+$ cations by seven and nine O atoms. The resulting coordination polyhedra of the two types of cations are highly distorted.

Related literature

For further information on this structure type, see: Friaa et al. (2003); Haj Abdallah & Haddad (2012). For background to the bond-valence method, see: Brown (2002).

Experimental

Crystal data

Na$_{1.67}$K$_{1.33}$Al$_3$(AsO$_4$)$_4$
M_r = 726.95
Orthorhombic, $Cmce$
a = 10.493 (1) Å
b = 20.395 (4) Å
c = 6.335 (4) Å
V = 1355.7 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 10.53 mm^{-1}
T = 293 K
0.40 × 0.10 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North et al., 1968)
T_{min} = 0.130, T_{max} = 0.332
1723 measured reflections
780 independent reflections
717 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
2 standard reflections every 120 min intensity decay: 1.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.112
S = 1.15
780 reflections
84 parameters
1 restraint
$\Delta\rho_{max}$ = 2.38 e Å^{-3}
$\Delta\rho_{min}$ = −1.33 e Å^{-3}

Table 1
Selected bond lengths (Å).

As1—O1	1.642 (5)	Al1—O5^{iii}	1.947 (3)
As1—O2^i	1.678 (3)	Al1—O5^{iv}	1.947 (3)
As1—O2	1.678 (3)	Al1—O5^i	1.947 (3)
As1—O3	1.694 (4)	Al1—O5	1.947 (3)
As2—O4^{ii}	1.648 (3)	Al2—O2^{ii}	1.817 (3)
As2—O4	1.648 (3)	Al2—O2^v	1.817 (3)
As2—O5	1.729 (3)	Al2—O4^v	1.924 (3)
As2—O5^{ii}	1.729 (3)	Al2—O4^{vi}	1.924 (3)
Al1—O3	1.827 (5)	Al2—O5^{ii}	1.991 (3)
Al1—O3^{iii}	1.827 (5)	Al2—O5	1.991 (3)

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

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, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2786).

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Brown, I. D. (2002). In *The Chemical Bond in Inorganic Chemistry: The Bond Valence Model*. Oxford University Press.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Friaa, B. B., Boughzala, H. & Jouini, T. (2003). *J. Solid State Chem.* **173**, 273–279.
Haj Abdallah, A. & Haddad, A. (2012). *Acta Cryst.* E**68**, i29.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

The aluminoarsenate Na$_{1.67}$K$_{1.33}$Al$_3$(AsO$_4$)$_4$

Mohamad Alem Bouhassine and Habib Boughzala

S1. Comment

Na$_{1.67}$K$_{1.33}$Al$_3$(AsO$_4$)$_4$ is isostructural with K$_3$Cr$_3$(AsO$_4$)$_4$ (Friaa *et al.* (2003)) and belongs to the $A^I M^{III}(XO_4)_4$ family of compounds (A^I = alkali metal, M^{III} = Al, Cr, Fe,.. X = As, P) . Its structure consists of AlO$_6$ octahedra and AsO$_4$ tetrahedra sharing corners and edges to form a two-dimensional framework (Fig.1) that consists of corrugated layers extending parallel to (010). Each layer lies on a *c*-glide plane perpendicular to the *b* axis at *y* = 0 and *y* = 1/2. In the asymmetric unit two AlO$_6$ octahedra are linked to an As1O$_4$ tetrahedron by sharing corners and to an As2O$_4$ tetrahedron by sharing edges. The alkali cations are occupationally disordered with occupancies of 0.725 (14), 0.112 (14), 0.314 (7) and 0.035 (12) for Na1, Na2, K1 and K2, leading to the chemical formula Na$_{1.67}$K$_{1.33}$Al$_3$(AsO$_4$)$_4$. Smaller than K$^+$, the seven- and nine-coordinated Na1$^+$ and Na2$^+$ (r$_{Na+}$ = 1.02 Å), are located in cavities surrounded by the anionic framework (Fig. 2). On the other hand, the K1$^+$ and K2$^+$ cations (r$_{K+}$ = 1.38 Å) are surrounded, respectively, by seven and six O atoms and are located in larger sites in the corrugated interlayer space. Using the bond valence method (Brown, 2002), the calculated bond-valence sum values (in valence units) of 5.17, 4.98, 3.04, 3.03, 0.86, 1.11, 0.92, 0.86, respectively, for As1, As2, Al1, Al2, Na1, Na2, K1 and K2 are in good agreement with the expected oxidation states.

A similar distribution of cations was observed in K$_{1.8}$Sr$_{0.6}$Al$_3$(AsO$_4$)$_4$ (Haj Abdallah *et al.*, 2012). In fact, smaller than K$^+$, the Sr^{2+} cations (r$_{Sr2+}$ = 1.18 Å) are located in the anionic cavities, on the other hand, K$^+$ occupy the interlayer space. The cationic distribution in these two structures make it reasonable to conclude that the interlayer space is reserved for bigger cations and the anionic cavities for smaller cations. To our knowledge, this is the first published structure with occupationally disordered alkali sites in the $A^I M^{III}(XO_4)_4$ family of compounds. Reports of some new members of this family will be published soon.

S2. Experimental

Crystals of Na$_{1.67}$K$_{1.33}$Al$_3$(AsO$_4$)$_4$ were obtained from a mixture of K$_2$CO$_3$, Al$_2$O$_3$ and NH$_4$H$_2$AsO$_4$ in the stoichiometric molar ratio K/Al/As=2/3/4. The mixture was finely ground and heated in a porcelain crucible at 723 K for 4 h to eliminate volatile products. The temperature was held at 1173 K during 10 days until fusion was reached. The sample was slowly cooled in a speed of 5 K/ h to 923 K and finally quenched to room temperature. A long wash with boiling water liberated colorless crystals. The qualitative analysis by electron microscope probe of a selected crystal revealed the presence of the different elements in the compound composition. It is most likely that the incorporated sodium stems from the crucible.

S3. Refinement

Except for K2 and Na2, both with a very low occupation, all atoms were refined with anisotropic displacement parameters. Constraints were applied to the Na$^+$ and K$^+$ cation occupation rates to achieve electro-neutrality. The highest and lowest values of the electron densities occurare located 0.97 Å and 0.80 Å, respectively, from As2.
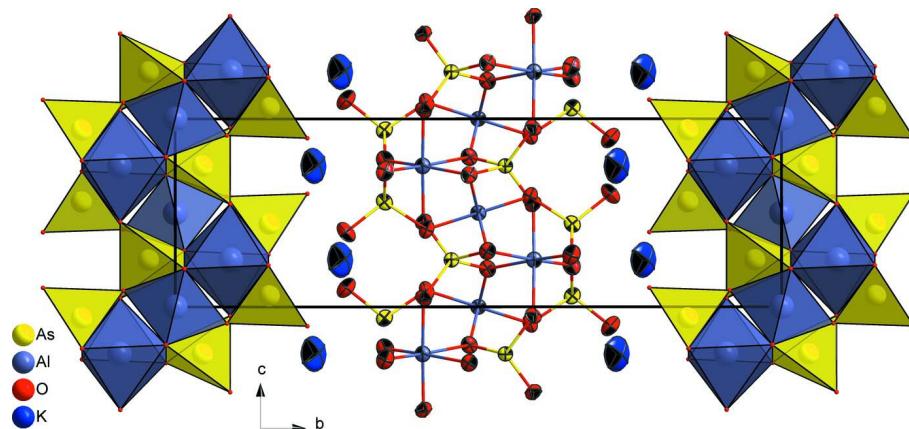
Figure 1

Projection of the $Na_{1.67}K_{1.33}Al_3(AsO_4)_4$ structure along [100], showing the $K1^+$ and $K2^+$ cations in the corrugated interlayer space. Displacement ellipsoids are drawn at the 90% probability level.
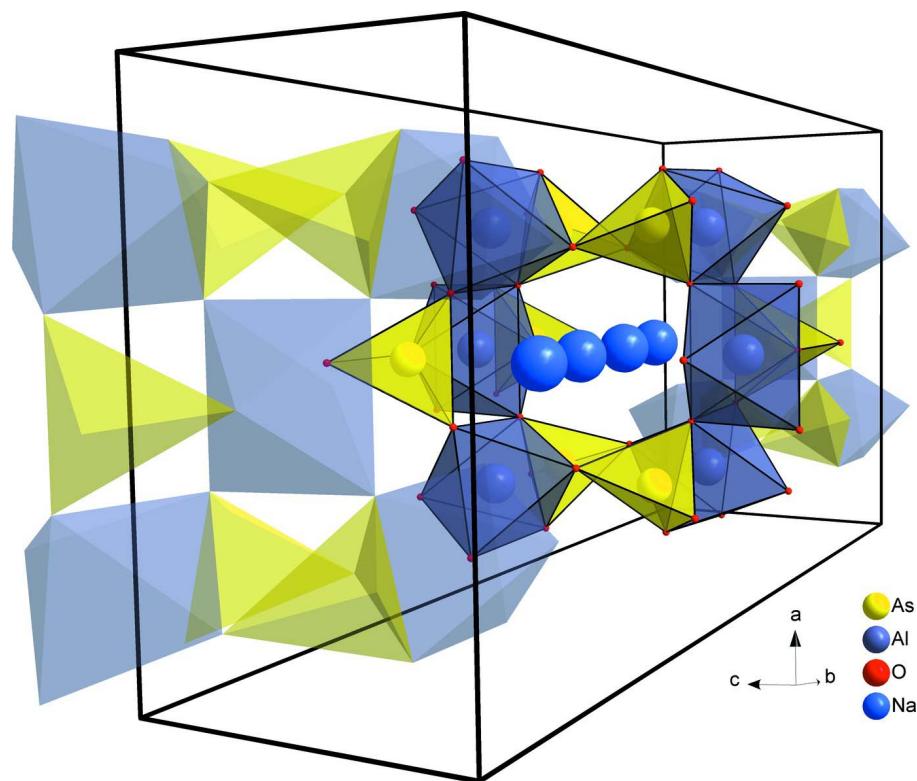
Figure 2

Cavities limited by the anionic framework hosting Na^+ cations in the $Na_{1.67}K_{1.33}Al_3(AsO_4)_4$ structure.

Sodium potassium trialuminium tetrakis(orthoarsenate)

Crystal data

$Na_{1.67}K_{1.33}Al_3(AsO_4)_4$	$a = 10.493\ (1)$ Å
$M_r = 726.95$	$b = 20.395\ (4)$ Å
Orthorhombic, $Cmce$	$c = 6.335\ (4)$ Å
Hall symbol: -C 2bc 2	$V = 1355.7\ (9)$ Å^3

$Z = 4$

$F(000) = 1370.4$

$D_x = 3.563$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 3.8–27°$

$\mu = 10.53$ mm^{-1}

$T = 293$ K

Plate, colourless

$0.40 \times 0.10 \times 0.07$ 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)

$T_{min} = 0.130$, $T_{max} = 0.332$

1723 measured reflections

780 independent reflections

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

$R_{int} = 0.062$

$\theta_{max} = 27.0°$, $\theta_{min} = 3.8°$

$h = -13 \rightarrow 1$

$k = -26 \rightarrow 1$

$l = -8 \rightarrow 8$

2 standard reflections every 120 min

intensity decay: 1.1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.112$

$S = 1.15$

780 reflections

84 parameters

1 restraint

Primary atom site location: structure-invariant
   direct methods

Secondary atom site location: difference Fourier
   map

$w = 1/[\sigma^2(F_o^2) + (0.0727P)^2 + 0.5867P]$
   where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 2.38$ e Å^{-3}

$\Delta\rho_{min} = -1.33$ e Å^{-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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
As1	0.0000	0.15486 (3)	0.05909 (10)	0.0075 (3)	
As2	0.2500	−0.04448 (3)	0.2500	0.0070 (3)	
Al1	0.0000	0.0000	0.0000	0.0063 (5)	
Al2	0.2500	0.09187 (10)	0.2500	0.0073 (4)	
O1	0.0000	0.2179 (3)	−0.1020 (8)	0.0163 (10)	
O2	0.1263 (3)	0.15363 (15)	0.2215 (5)	0.0110 (7)	
O3	0.0000	0.0854 (2)	−0.0873 (7)	0.0095 (9)	
O4	0.2105 (3)	−0.09062 (16)	0.4534 (4)	0.0102 (6)	
O5	0.1364 (3)	0.01511 (13)	0.2027 (5)	0.0086 (6)	
Na1	0.0000	0.1628 (3)	0.5513 (7)	0.0350 (18)	0.725 (14)
Na2	0.0000	0.0635 (17)	0.520 (5)	0.042 (12)*	0.112 (14)

K1	0.2125 (6)	0.2737 (3)	0.1075 (10)	0.048 (2)	0.314 (7)
K2	0.2500	0.271 (3)	0.2500	0.03 (2)*	0.035 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.0016 (4)	0.0103 (4)	0.0108 (4)	0.000	0.000	0.0013 (2)
As2	0.0039 (4)	0.0086 (4)	0.0084 (4)	0.000	−0.0005 (2)	0.000
Al1	0.0011 (10)	0.0090 (12)	0.0089 (11)	0.000	0.000	0.0003 (10)
Al2	0.0028 (9)	0.0093 (9)	0.0099 (9)	0.000	−0.0001 (6)	0.000
O1	0.020 (3)	0.013 (2)	0.016 (2)	0.000	0.000	0.006 (2)
O2	0.0045 (15)	0.0124 (15)	0.0161 (15)	0.0010 (11)	−0.0040 (13)	−0.0019 (11)
O3	0.006 (2)	0.009 (2)	0.0133 (19)	0.000	0.000	−0.0024 (17)
O4	0.0091 (15)	0.0116 (15)	0.0100 (13)	−0.0029 (12)	0.0009 (12)	0.0017 (11)
O5	0.0033 (14)	0.0105 (15)	0.0120 (13)	0.0023 (11)	−0.0018 (13)	−0.0007 (10)
Na1	0.037 (3)	0.047 (3)	0.020 (3)	0.000	0.000	−0.0033 (19)
K1	0.053 (3)	0.034 (3)	0.059 (4)	−0.029 (3)	0.013 (3)	0.003 (2)

Geometric parameters (Å, º)

As1—O1	1.642 (5)	O4—Na2^{xv}	2.284 (9)
As1—O2ⁱ	1.678 (3)	O4—Na1^{xv}	2.655 (4)
As1—O2	1.678 (3)	O4—K1^{xvi}	2.795 (6)
As1—O3	1.694 (4)	O4—K2^{xvi}	3.13 (5)
As2—O4ⁱⁱ	1.648 (3)	O5—Na2	2.66 (3)
As2—O4	1.648 (3)	O5—Na2^{xv}	2.77 (3)
As2—O5	1.729 (3)	Na1—Na2	2.03 (4)
As2—O5ⁱⁱ	1.729 (3)	Na1—O1^{xvii}	2.467 (7)
As2—Al2	2.781 (2)	Na1—O2ⁱ	2.481 (5)
Al1—O3	1.827 (5)	Na1—K1^{viii}	2.603 (8)
Al1—O3ⁱⁱⁱ	1.827 (5)	Na1—K1^{xviii}	2.603 (8)
Al1—O5ⁱⁱⁱ	1.947 (3)	Na1—O1^{xviii}	2.619 (8)
Al1—O5^{iv}	1.947 (3)	Na1—O4^{xv}	2.655 (4)
Al1—O5ⁱ	1.947 (3)	Na1—O4^{vi}	2.655 (4)
Al1—O5	1.947 (3)	Na1—O3^{xvii}	2.781 (7)
Al2—O2ⁱⁱ	1.817 (3)	Na1—K2^{xix}	3.21 (2)
Al2—O2	1.817 (3)	Na2—O4^{vi}	2.284 (9)
Al2—O4^v	1.924 (3)	Na2—O4^{xv}	2.284 (9)
Al2—O4^{vi}	1.924 (3)	Na2—O3^{xvii}	2.53 (3)
Al2—O5ⁱⁱ	1.991 (3)	Na2—Na2^{xv}	2.60 (7)
Al2—O5	1.991 (3)	Na2—O5ⁱ	2.66 (3)
Al2—Na2	3.19 (2)	Na2—O5^{vi}	2.77 (3)
Al2—Na2^{vii}	3.19 (2)	Na2—O5^{xv}	2.77 (3)
Al2—Na1^{vii}	3.552 (3)	Na2—O2ⁱ	2.95 (3)
Al2—Na1	3.552 (3)	Na2—As2^{xiv}	3.025 (17)
Al2—K1^{viii}	3.579 (6)	K1—K2	0.986 (7)
O1—Na1^{ix}	2.467 (7)	K1—K1^{xi}	1.846 (12)
O1—Na1^x	2.620 (8)	K1—K1ⁱⁱ	1.969 (14)

O1—K2^{x}	2.795 (5)	K1—K2^{xi}	2.47 (2)
O1—K2^{xi}	2.795 (5)	K1—Na1^{x}	2.603 (8)
O1—K1^{i}	2.833 (7)	K1—O4^{xx}	2.795 (6)
O1—K1	2.833 (7)	K1—O1^{xviii}	2.896 (6)
O1—K1^{x}	2.896 (6)	K1—O2^{xii}	2.999 (7)
O1—K1^{xii}	2.896 (6)	K1—O1^{xi}	3.022 (6)
O1—K1^{xi}	3.022 (6)	K1—O2^{xi}	3.067 (6)
O1—K1^{xiii}	3.022 (6)	K2—K1^{ii}	0.986 (7)
O2—Na1	2.481 (5)	K2—K1^{viii}	2.47 (2)
O2—K1	2.708 (6)	K2—K1^{xi}	2.47 (2)
O2—K2	2.73 (5)	K2—O2^{ii}	2.73 (5)
O2—Na2	2.95 (3)	K2—O1^{xi}	2.795 (5)
O2—K1^{viii}	2.999 (7)	K2—O1^{xviii}	2.795 (5)
O2—K1^{xi}	3.067 (6)	K2—O4^{xx}	3.13 (5)
O2—K1^{ii}	3.166 (7)	K2—O4^{xxi}	3.13 (5)
O3—Na2^{ix}	2.53 (3)	K2—Na1^{x}	3.21 (2)
O3—Na1^{ix}	2.781 (7)	K2—Na1^{xix}	3.21 (2)
O4—Al2^{xiv}	1.924 (3)		
O1—As1—O2^{i}	113.13 (15)	O4^{xv}—Na2—O2	109.3 (12)
O1—As1—O2	113.13 (15)	O3^{xvii}—Na2—O2	121.4 (11)
O2^{i}—As1—O2	104.3 (2)	Na2^{xv}—Na2—O2	123.8 (17)
O1—As1—O3	108.4 (3)	O5^{i}—Na2—O2	89.3 (10)
O2^{i}—As1—O3	108.86 (14)	O5—Na2—O2	60.3 (6)
O2—As1—O3	108.86 (14)	O5^{vi}—Na2—O2	122.25 (12)
O4^{ii}—As2—O4	110.4 (2)	O5^{xv}—Na2—O2	175.4 (8)
O4^{ii}—As2—O5	116.04 (14)	O2^{i}—Na2—O2	53.4 (6)
O4—As2—O5	111.32 (15)	Na1—Na2—As2^{xiv}	94.7 (8)
O4^{ii}—As2—O5^{ii}	111.32 (15)	O4^{vi}—Na2—As2^{xiv}	32.5 (3)
O4—As2—O5^{ii}	116.04 (14)	O4^{xv}—Na2—As2^{xiv}	146.6 (14)
O5—As2—O5^{ii}	90.65 (19)	O3^{xvii}—Na2—As2^{xiv}	63.2 (6)
O4^{ii}—As2—Al2	124.81 (11)	Na2^{xv}—Na2—As2^{xiv}	85.4 (10)
O4—As2—Al2	124.81 (11)	O5^{i}—Na2—As2^{xiv}	141.6 (11)
O5—As2—Al2	45.33 (10)	O5—Na2—As2^{xiv}	81.4 (3)
O5^{ii}—As2—Al2	45.33 (10)	O5^{vi}—Na2—As2^{xiv}	34.3 (3)
O3—Al1—O3^{iii}	180.0	O5^{xv}—Na2—As2^{xiv}	93.9 (10)
O3—Al1—O5^{iii}	87.19 (13)	O2^{i}—Na2—As2^{xiv}	141.0 (10)
O3^{iii}—Al1—O5^{iii}	92.81 (13)	O2—Na2—As2^{xiv}	89.9 (4)
O3—Al1—O5^{iv}	87.19 (13)	O2—K1—O4^{xx}	158.4 (3)
O3^{iii}—Al1—O5^{iv}	92.81 (13)	K2—K1—O1	136 (2)
O5^{iii}—Al1—O5^{iv}	94.60 (18)	K1^{xi}—K1—O1	77.3 (4)
O3—Al1—O5^{i}	92.80 (13)	K1^{ii}—K1—O1	138.1 (3)
O3^{iii}—Al1—O5^{i}	87.20 (13)	K2^{xi}—K1—O1	63.1 (4)
O5^{iii}—Al1—O5^{i}	85.40 (18)	Na1^{x}—K1—O1	57.43 (19)
O5^{iv}—Al1—O5^{i}	180.0	O2—K1—O1	59.97 (16)
O3—Al1—O5	92.80 (13)	O4^{xx}—K1—O1	109.1 (3)
O3^{iii}—Al1—O5	87.19 (13)	K2—K1—O1^{xviii}	74.3 (4)
O5^{iii}—Al1—O5	180.0	K1^{xi}—K1—O1^{xviii}	145.9 (4)

O5^{iv}—Al1—O5	85.40 (18)	K1^{ii}—K1—O1^{xviii}	74.1 (3)
O5^{i}—Al1—O5	94.60 (18)	K2^{xi}—K1—O1^{xviii}	136.6 (5)
O2^{ii}—Al2—O2	92.3 (2)	Na1^{x}—K1—O1^{xviii}	53.00 (18)
O2^{ii}—Al2—O4^{v}	87.27 (15)	O2—K1—O1^{xviii}	68.10 (17)
O2—Al2—O4^{v}	93.78 (15)	O4^{xx}—K1—O1^{xviii}	91.3 (2)
O2^{ii}—Al2—O4^{vi}	93.78 (15)	O1—K1—O1^{xviii}	73.48 (15)
O2—Al2—O4^{vi}	87.27 (15)	K2—K1—O2^{xii}	153 (3)
O4^{v}—Al2—O4^{vi}	178.5 (2)	K1^{xi}—K1—O2^{xii}	77.6 (4)
O2^{ii}—Al2—O5^{ii}	95.88 (12)	K1^{ii}—K1—O2^{xii}	150.20 (12)
O2—Al2—O5^{ii}	171.00 (15)	K2^{xi}—K1—O2^{xii}	59.0 (10)
O4^{v}—Al2—O5^{ii}	90.44 (14)	Na1^{x}—K1—O2^{xii}	51.99 (17)
O4^{vi}—Al2—O5^{ii}	88.37 (14)	O2—K1—O2^{xii}	124.3 (2)
O2^{ii}—Al2—O5	171.00 (15)	O4^{xx}—K1—O2^{xii}	52.81 (14)
O2—Al2—O5	95.89 (12)	O1—K1—O2^{xii}	65.11 (18)
O4^{v}—Al2—O5	88.37 (14)	O1^{xviii}—K1—O2^{xii}	104.9 (3)
O4^{vi}—Al2—O5	90.44 (14)	K2—K1—O1^{xi}	67.3 (4)
O5^{ii}—Al2—O5	76.27 (18)	K1^{xi}—K1—O1^{xi}	66.1 (4)
O2^{ii}—Al2—As2	133.87 (11)	K1^{ii}—K1—O1^{xi}	67.1 (3)
O2—Al2—As2	133.87 (11)	K2^{xi}—K1—O1^{xi}	81.5 (2)
O4^{v}—Al2—As2	89.24 (12)	Na1^{x}—K1—O1^{xi}	145.6 (2)
O4^{vi}—Al2—As2	89.24 (12)	O2—K1—O1^{xi}	112.8 (3)
O5^{ii}—Al2—As2	38.14 (9)	O4^{xx}—K1—O1^{xi}	87.10 (17)
O5—Al2—As2	38.14 (9)	O1—K1—O1^{xi}	143.4 (2)
As1—O2—Al2	129.43 (18)	O1^{xviii}—K1—O1^{xi}	140.6 (2)
As1—O3—Al1	129.2 (3)	O2^{xii}—K1—O1^{xi}	105.27 (19)
As2—O4—Al2^{xiv}	135.8 (2)	K2—K1—O2^{xi}	115.2 (17)
As2—O5—Al1	120.66 (15)	K1^{xi}—K1—O2^{xi}	61.0 (3)
As2—O5—Al2	96.54 (14)	K1^{ii}—K1—O2^{xi}	113.7 (4)
Al1—O5—Al2	131.59 (15)	K2^{xi}—K1—O2^{xi}	57.9 (10)
O2—Na1—O3^{xvii}	130.6 (2)	Na1^{x}—K1—O2^{xi}	98.0 (2)
K1^{viii}—Na1—O3^{xvii}	99.79 (19)	O2—K1—O2^{xi}	143.4 (2)
K1^{xviii}—Na1—O3^{xvii}	99.79 (19)	O4^{xx}—K1—O2^{xi}	55.33 (12)
O1^{xviii}—Na1—O3^{xvii}	146.4 (2)	O1—K1—O2^{xi}	108.0 (2)
O4^{xv}—Na1—O3^{xvii}	72.21 (14)	O1^{xviii}—K1—O2^{xi}	145.9 (3)
O4^{vi}—Na1—O3^{xvii}	72.21 (14)	O2^{xii}—K1—O2^{xi}	51.17 (15)
Na2—Na1—As1	81.5 (10)	O1^{xi}—K1—O2^{xi}	54.13 (14)
O1^{xvii}—Na1—As1	155.8 (3)	K1^{ii}—K2—K1	174 (6)
O2^{i}—Na1—As1	32.36 (9)	K1^{ii}—K2—K1^{viii}	40.9 (15)
O2—Na1—As1	32.36 (9)	K1—K2—K1^{viii}	142 (2)
K1^{viii}—Na1—As1	99.35 (18)	K1^{ii}—K2—K1^{xi}	142 (2)
K1^{xviii}—Na1—As1	99.35 (18)	K1—K2—K1^{xi}	40.9 (15)
O1^{xviii}—Na1—As1	71.20 (16)	K1^{viii}—K2—K1^{xi}	137 (2)
O4^{xv}—Na1—As1	87.71 (12)	K1^{ii}—K2—O2	107 (3)
O4^{vi}—Na1—As1	87.71 (12)	K1—K2—O2	78 (3)
O3^{xvii}—Na1—As1	142.4 (2)	K1^{viii}—K2—O2	70.1 (11)
Na2—Na1—K2^{xix}	117.1 (10)	K1^{xi}—K2—O2	72.0 (11)
O1^{xvii}—Na1—K2^{xix}	57.3 (3)	K1^{ii}—K2—O2^{ii}	78 (3)
O2^{i}—Na1—K2^{xix}	143.1 (5)	K1—K2—O2^{ii}	107 (3)

Angle	Value	Angle	Value
O2—Na1—K2[xix]	85.70 (14)	K1[viii]—K2—O2[ii]	72.0 (11)
K1[viii]—Na1—K2[xix]	15.5 (4)	K1[xi]—K2—O2[ii]	70.1 (11)
K1[xviii]—Na1—K2[xix]	116.0 (8)	O2—K2—O2[ii]	57.3 (11)
O1[xviii]—Na1—K2[xix]	75.8 (9)	K1[ii]—K2—O1[xi]	85.9 (5)
O4[xv]—Na1—K2[xix]	156.7 (5)	K1—K2—O1[xi]	93.7 (5)
O4[vi]—Na1—K2[xix]	63.7 (8)	K1[viii]—K2—O1[xi]	119.1 (6)
O3[xvii]—Na1—K2[xix]	85.1 (6)	K1[xi]—K2—O1[xi]	64.7 (2)
As1—Na1—K2[xix]	114.45 (17)	O2—K2—O1[xi]	119.6 (16)
Na1—Na2—O4[vi]	75.6 (9)	O2[ii]—K2—O1[xi]	69.3 (6)
Na1—Na2—O4[xv]	75.6 (9)	K1[ii]—K2—O1[xviii]	93.7 (5)
O4[vi]—Na2—O4[xv]	150.7 (17)	K1—K2—O1[xviii]	85.9 (5)
Na1—Na2—O3[xvii]	74.3 (11)	K1[viii]—K2—O1[xviii]	64.7 (2)
O4[vi]—Na2—O3[xvii]	83.4 (9)	K1[xi]—K2—O1[xviii]	119.1 (6)
O4[xv]—Na2—O3[xvii]	83.4 (9)	O2—K2—O1[xviii]	69.3 (6)
Na1—Na2—Na2[xv]	180 (2)	O2[ii]—K2—O1[xviii]	119.6 (16)
O4[vi]—Na2—Na2[xv]	104.4 (9)	O1[xi]—K2—O1[xviii]	171 (2)
O4[xv]—Na2—Na2[xv]	104.4 (9)	K1[ii]—K2—O4[xx]	113 (4)
O3[xvii]—Na2—Na2[xv]	105.8 (19)	K1—K2—O4[xx]	62 (3)
Na1—Na2—O5[i]	116.3 (13)	K1[viii]—K2—O4[xx]	133.6 (15)
O4[vi]—Na2—O5[i]	131.8 (13)	K1[xi]—K2—O4[xx]	88.7 (8)
O4[xv]—Na2—O5[i]	67.9 (5)	O2—K2—O4[xx]	134.51 (15)
O3[xvii]—Na2—O5[i]	144.1 (7)	O2[ii]—K2—O4[xx]	151.78 (16)
Na2[xv]—Na2—O5[i]	63.6 (11)	O1[xi]—K2—O4[xx]	85.1 (10)
Na1—Na2—O5	116.3 (13)	O1[xviii]—K2—O4[xx]	86.7 (10)
O4[vi]—Na2—O5	67.9 (5)	K1[ii]—K2—O4[xxi]	62 (3)
O4[xv]—Na2—O5	131.8 (13)	K1—K2—O4[xxi]	113 (4)
O3[xvii]—Na2—O5	144.1 (7)	K1[viii]—K2—O4[xxi]	88.7 (8)
Na2[xv]—Na2—O5	63.6 (11)	K1[xi]—K2—O4[xxi]	133.6 (15)
O5[i]—Na2—O5	65.1 (8)	O2—K2—O4[xxi]	151.78 (16)
Na1—Na2—O5[vi]	120.9 (12)	O2[ii]—K2—O4[xxi]	134.51 (15)
O4[vi]—Na2—O5[vi]	66.1 (5)	O1[xi]—K2—O4[xxi]	86.7 (10)
O4[xv]—Na2—O5[vi]	126.3 (13)	O1[xviii]—K2—O4[xxi]	85.1 (10)
O3[xvii]—Na2—O5[vi]	58.6 (7)	O4[xx]—K2—O4[xxi]	51.3 (9)
Na2[xv]—Na2—O5[vi]	59.2 (11)	K1[ii]—K2—Na1[x]	132 (2)
O5[i]—Na2—O5[vi]	122.8 (13)	K1—K2—Na1[x]	45.0 (15)
O5—Na2—O5[vi]	89.2 (7)	K1[viii]—K2—Na1[x]	112.6 (2)
Na1—Na2—O5[xv]	120.9 (12)	K1[xi]—K2—Na1[x]	85.8 (3)
O4[vi]—Na2—O5[xv]	126.3 (13)	O2—K2—Na1[x]	87.4 (4)
O4[xv]—Na2—O5[xv]	66.1 (5)	O2[ii]—K2—Na1[x]	141.5 (14)
O3[xvii]—Na2—O5[xv]	58.6 (7)	O1[xi]—K2—Na1[x]	127.1 (11)
Na2[xv]—Na2—O5[xv]	59.2 (11)	O1[xviii]—K2—Na1[x]	48.0 (3)
O5[i]—Na2—O5[xv]	89.2 (7)	O4[xx]—K2—Na1[x]	49.6 (6)
O5—Na2—O5[xv]	122.8 (13)	O4[xxi]—K2—Na1[x]	83.8 (12)
O5[vi]—Na2—O5[xv]	62.1 (8)	K1[ii]—K2—Na1[xix]	45.0 (15)
Na1—Na2—O2[i]	56.1 (8)	K1—K2—Na1[xix]	132 (2)
O4[vi]—Na2—O2[i]	109.3 (12)	K1[viii]—K2—Na1[xix]	85.8 (3)
O4[xv]—Na2—O2[i]	57.4 (6)	K1[xi]—K2—Na1[xix]	112.6 (2)
O3[xvii]—Na2—O2[i]	121.4 (11)	O2—K2—Na1[xix]	141.5 (14)

Na2^{xv}—Na2—O2^{i}	123.8 (17)	O2^{ii}—K2—Na1^{xix}	87.4 (4)
O5^{i}—Na2—O2^{i}	60.3 (6)	O1^{xi}—K2—Na1^{xix}	48.0 (3)
O5—Na2—O2^{i}	89.3 (10)	O1^{xviii}—K2—Na1^{xix}	127.1 (11)
O5^{vi}—Na2—O2^{i}	175.4 (8)	O4^{xx}—K2—Na1^{xix}	83.8 (12)
O5^{xv}—Na2—O2^{i}	122.25 (12)	O4^{xxi}—K2—Na1^{xix}	49.6 (6)
Na1—Na2—O2	56.1 (8)	Na1^{x}—K2—Na1^{xix}	130.3 (18)
O4^{vi}—Na2—O2	57.4 (6)		

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