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$Na_7Al_3(As_2O_7)_4$

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ(Al–O) = 0.004 Å; disorder in main residue; R factor = 0.034; wR factor = 0.085; data-to-parameter ratio = 11.7.

The title compound, heptasodium trialuminium tetrakis(diarsenate), has been isolated as single crystals from a solid-state reaction. Its structure, which is isotypic with that of the $Na_7Fe_3(X_2O_7)_4$ (X = As, P) family of compounds, consists of AlO_6 octahedra sharing their vertices with As_2O_7 groups, forming a three-dimensional $[Al_3(As_2O_7)_4]_\infty$ framework incorporating channels occupied by the sodium ions. One of the aluminium ions lies on a crystallographic twofold axis. The sodium ions are situated over ten positions (one with site symmetry 2), all but one of which are partially occupied.

Related literature

For isotopic compounds, see: Masquelier & d'Yvoire (1991); Masquelier *et al.* (1990, 1994); Quarez *et al.*(2009, 2010). For bond lengths and angles in related structures, see: Driss & Jouini (1994); Masquelier *et al.* (1995). For structural relationships, see: Lii *et al.* (1989); Hwu & Willis (1991); Boughzala *et al.* (1993); Boughzala & Jouini (1995); Lin & Lii (1996); Fukuoka *et al.* (2003); Ouerfelli *et al.* (2007). For bond-valence parameters, see: Brown & Altermatt (1985).

Experimental

Crystal data

$Na_7Al_3(As_2O_7)_4$
M_r = 1289.23
Monoclinic, $C2/c$
a = 9.800 (1) Å
b = 8.468 (1) Å
c = 28.637 (2) Å
β = 94.14 (1)°
V = 2370.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 11.50 mm^{-1}
T = 298 K
0.25 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min}$ = 0.759, $T_{\max}$ = 0.891
3958 measured reflections
2583 independent reflections
2150 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.056
2 standard reflections every 120 min intensity decay: 1.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.085
S = 1.10
2583 reflections
221 parameters
$\Delta\rho_{\max}$ = 1.27 e Å^{-3}
$\Delta\rho_{\min}$ = −0.98 e Å^{-3}

Table 1
Selected bond lengths (Å).

Al1—O12$^{\rm i}$	1.906 (4)	As1—O3	1.689 (4)
Al1—O12	1.906 (4)	As1—O4	1.776 (4)
Al1—O1$^{\rm ii}$	1.932 (4)	As2—O13	1.638 (4)
Al1—O1$^{\rm iii}$	1.932 (4)	As2—O14	1.675 (4)
Al1—O3	1.994 (4)	As2—O12	1.686 (4)
Al1—O3$^{\rm i}$	1.994 (4)	As2—O4	1.769 (4)
Al2—O14	1.920 (4)	As3—O7	1.668 (4)
Al2—O10$^{\rm iv}$	1.933 (4)	As3—O5	1.671 (4)
Al2—O7$^{\rm iv}$	1.942 (4)	As3—O6	1.677 (4)
Al2—O5	1.947 (4)	As3—O11	1.736 (4)
Al2—O9$^{\rm v}$	1.955 (4)	As4—O8	1.646 (4)
Al2—O6$^{\rm ii}$	2.000 (4)	As4—O10	1.676 (4)
As1—O2	1.651 (4)	As4—O9	1.679 (4)
As1—O1	1.676 (4)	As4—O11	1.760 (4)

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

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); 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, 2012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7105).

References

Boughzala, H., Driss, A. & Jouini, T. (1993). *Acta Cryst.* C**49**, 425–427.
Boughzala, H. & Jouini, T. (1995). *Acta Cryst.* C**51**, 179–181.
Brandenburg, K. (1998). *DIAMOND*. University of Bonn, Germany.
Brown, I. D. & Altermatt, D. (1985). *Acta Cryst.* B**41**, 244–247.
Driss, A. & Jouini, T. (1994). *J. Solid State Chem.* **112**, 277–280.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Fukuoka, H., Matsunaga, H. & Yamanaka, S. (2003). *Mater. Res. Bull.* **38**, 991–1001.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Hwu, S.-J. & Willis, E. D. (1991). *J. Solid State Chem.* **93**, 69–76.
Lii, K. H., Chen, J. J. & Wang, S. L. (1989). *J. Solid State Chem.* **78**, 178–183.
Lin, K.-J. & Lii, K.-H. (1996). *Acta Cryst.* C**52**, 2387–2389.
Macíček, J. & Yordanov, A. (1992). *J. Appl. Cryst.* **25**, 73–80.
Masquelier, C. & d'Yvoire, F. (1991). *J. Solid State Chem.* **95**, 156–167.
Masquelier, C., d'Yvoire, F., Bretey, E., Berthet, P. & Peytour-Chansac, C. (1994). *Solid State Ionics*, **67**, 183–189.
Masquelier, C., d'Yvoire, F. & Collin, G. (1995). *J. Solid State Chem.* **118**, 33–44.
Masquelier, C., d'Yvoire, F. & Rodier, N. (1990). *Acta Cryst.* C**46**, 1584–1587.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ouerfelli, N., Guesmi, A., Mazza, D., Madani, A., Zid, M. F. & Driss, A. (2007). *J. Solid State Chem.* **180**, 1224–1229.
Quarez, E., Mentré, O., Oumellala, Y. & Masquelier, C. (2009). *New J. Chem.* **33**, 998–1005.
Quarez, E., Mentré, O., Oumellala, Y. & Masquelier, C. (2010). *New J. Chem.* **34**, 287–293.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

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$Na_7Al_3(As_2O_7)_4$

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S1. Comment

A new family of compounds $Na_7M_3(X_2O_7)_4$ (M = Fe, Al, Cr, Ga; X = P, As) studied by Masquelier *et al.* (1994) present interesting ion conductivity properties. In this family line, a structural study was carried out only for $Na_7Fe_3(As_2O_7)_4$ and $Na_7Fe_3(P_2O_7)_4$ compounds by Masquelier *et al.*(1990, 1991). In addition, another structural study was conducted to isotypes compounds $Na_5Ag_2Fe_3(As_2O_7)_4$ and $Na_2Ag_5Fe_3(P_2O_7)_4$ by Quarez *et al.* (2009). Also, electrical measurements were also made by Quarez *et al.* (2009) for $Ag_7Fe_3(X_2O_7)_4$ (X = As, P) compounds. However, as for the $Na_7Al_3(As_2O_7)_4$ compound no structural analysis has been reported so far.

The structure of compound $Na_7Al_3(As_2O_7)_4$ shows a three-dimensional anionic framework $[Al_3(As_2O_7)\ _4]_\infty$ composed of octahedron AlO_6 sharing vertices with As_2O_7 groups. This framework defines the interstitial spaces in which the Na^+ ions are located in a partially disordered distribution to ensure the electrical neutrality. The single unit $[Al_3(As_2O_7)_4]^{7-}$ consists of an octahedron $Al1O_6$ and two octahedra $Al2O_6$ related to As_2O_7 group by sharing vertices (Fig. 1). The two aluminium atoms occupy two crystallographically independent sites: the aluminium Al1 is in special position 4e of a symmetry equal to 2; whereas the Al2 is in general position of 8f. In this unit, the connection between the octahedra $Al1O_6$ and $Al2O_6$ is provided by the group $As1As2O_7$ through oxygen atom O14. In this structure, the units $[Al_3(As_2O_7)_4]^{7-}$ are inter-related thanks to composite bridges of types Al—O—As and As—O—Al respectively. These bridges are located between the octahedra AlO_6 and As_2O_7 diarsenates groups in order to handle two types of parallel layers to the (a, b) plan. According to (010) (Fig. 2), a projection of the structure shows that the anionic framework consists of a succession of layers as follow: A: $[Al1(As2As3O_7)_2]_\infty$ and B: $[(Al2As3As4O_7)_2]_\infty$ perpendicular to c alternately. In the layers A, the only components are Octahedra $Al1O_6$, whereas other aluminium octahedra $Al2O_6$ shape layers B.

On the one hand, in the layer A, each octahedron $Al1O_6$ is connected to two groups $As1As2O_7$ by sharing both a vertex and two other groups $As1As2O_7$ such as the $Al1O_6$ octahedron shares two of its vertices with the same group As_2O_7. By rotation around the fold axis, these groups are equivalent (Fig. 3). This mode of connection is found in phosphates: $ARu_2(P_2O_7)_2$ (A = Li, Na, Ag) (Fukuoka *et al.*, 2003.), $NaMo_2(P_2O_7)_2$ (Hwu *et al.*, 1991), and $SrV_2(P_2O_7)_2$ (Lii *et al.*, 1989).

On the other hand, in the layer B, each octahedron $Al2O_6$ is connected to four As_2O_7 groups through the formation of composite bridges Al—O—As and the division of two vertices with a fifth group As_2O_7 (Fig. 3). This layer is formed by $AlAs_2O_{11}$ units related through the formation of Al—O—As composed bridges. This type of M—O—As bond between MAs_2O_{11} units (M = Al, Ga, Fe) is situated in the following isostructural compounds: $RbAlAs_2O_7$ (Boughzala *et al.*, 1993), $KAlAs_2O_7$ (Boughzala *et al.*, 1995), $KGaAs_2O_7$ (Lin *et al.*, 1996) and $TlFe_{0.22}Al_{0.78}As_2O_7$ (Ouerfelli *et al.*, 2007).

The O14 oxygen atom guarantees the bond between the layers A and B through the bridges Al2—O14—As2.

The anionic framework $[Al_3(As_2O_7)_4]_\infty$ can be also described as alternate stacking of octahedral AlO_6 layers and As_2O_7 groups layers parallel to $(\bar{1}01)$ (Fig. 4).

In this structure, the sodium ions are distributed through ten crystallographic sites in the interstices of the anionic network. The first type of the site corresponding to 8f position is totally occupied by the Na1 cation which is localized in the layer B. As for the nine other sites, they are partially occupied. And these can be arranged into groups of three sets: (Na2A—Na2B—Na2C), (Na3A—Na3B) and (Na4A—Na4B—Na4C—Na4D). Different sites of the same group are too close to be occupied simultaneously. As a result, the total number of Na^+ ions for each group is less than or equal to one. These sodium ions are predominantly located in the layer A and they are distributed in the vicinity of two plans parallel to (001) respectively to dimensions $z \simeq 0.15$ and $z \simeq 0.35$. Also, the Na2B site, located on the binary axis, occupies an intermediate position ($z = 1/4$). Examination of geometric factors in the structure shows that they are in accordance with those found in the literature (Driss *et al.*, 1994; Masquelier *et al.*, 1995.). In addition, the use of the BVS method for the calculation of different valences of bonds, using the empirical formula of Brown (Brown & Altermatt, 1985), does satisfy the expected values of ion charge: Al1 (2.73), Al2 (2.69), As1 (4.90), As2 (4.98), As3 (5.01), As4 (5.00), Na1 (1.16), Na2A (0.87), Na2B (1.13), Na2C (0.79), Na3A (1.00), Na3B (1.03), Na4A (0.97), Na4B (0.95), Na4C (1.01), Na4D (0, 93). In order to use these structural data and to connect them to the physicochemical properties, especially ion-conducting electrical measurements through a complex impedance bridge are in progress.

S2. Experimental

The crystals related to the $Na_7Al_3(As_2O_7)_4$ phase were obtained from reactants: $NaHCO_3$ (Prolabo, 27778), Al_2O_3 (Riedel-de Haen, 167305) $NH_4H_2AsO_4$ (prepared in the laboratory, JCPDS-775), taken in molar proportions: Na: A l: As = 10: 1: 9. Finely ground, the mixture was put in a porcelain crucible, placed in an oven and preheated in air at 673 K for 24 h to remove volatiles. After that, the mixture is raised to a synthesis temperature close to the melting 968 K through stages of 100 degrees followed by grinding. The mixture is then left at this temperature for a week to promote germination and growth of crystals. The final residue undergoes a first slow cooling (5 ° / half day, at 800 K) and a second fast (50 ° / h) to room temperature. Transparent crystals of prismatic form, clear outline and sufficient size for measurements of intensities, have been separated from the stream by successive hot water washes.

S3. Refinement

The collection was carried out in the monoclinic system of C2 / c space group. During the final refinement and for electrical neutrality reasons, the occupancy rate of Na^+ cations were conducted using the SUMP condition authorized by the *SHELXL* program. The refinement of all variable parameters leads to well defined ellipsoids. The maximum and minimum densities of electrons remaining in the Fourier-difference are respectively situated at 0.86 Å from the As4 site and at 1.35 Å from the NA3B site.

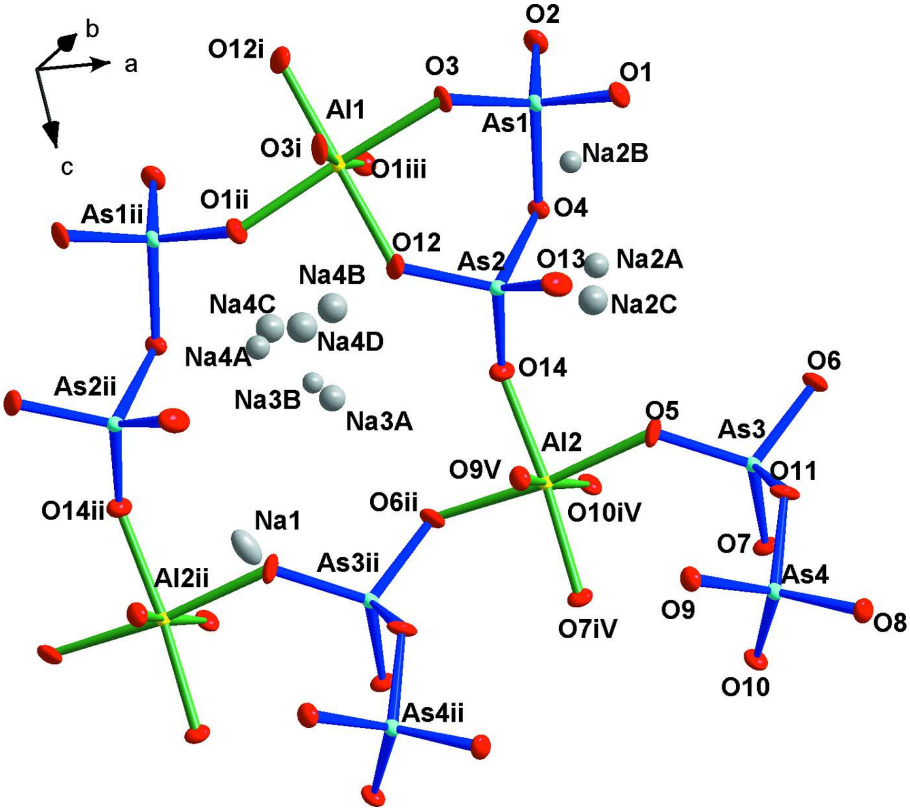

Figure 1

Part of Na_7Al_3 $(As2O_7)$ $_4$ structure. The ellipsoids were defined with 50% probability. [Symmetry code: (i): - *x*, *y*, - *z* + 0.5; (ii): *x* - 1/2, *y* - 1/2, *z*; (iii): - *x* + 1/2, *y* - 1/2, - *z* + 0.5; (iv): - *x* + 1, - *y*, - *z* + 1; (v): -*x* + 1/2, - *y* + 1/2, - *z* + 1].

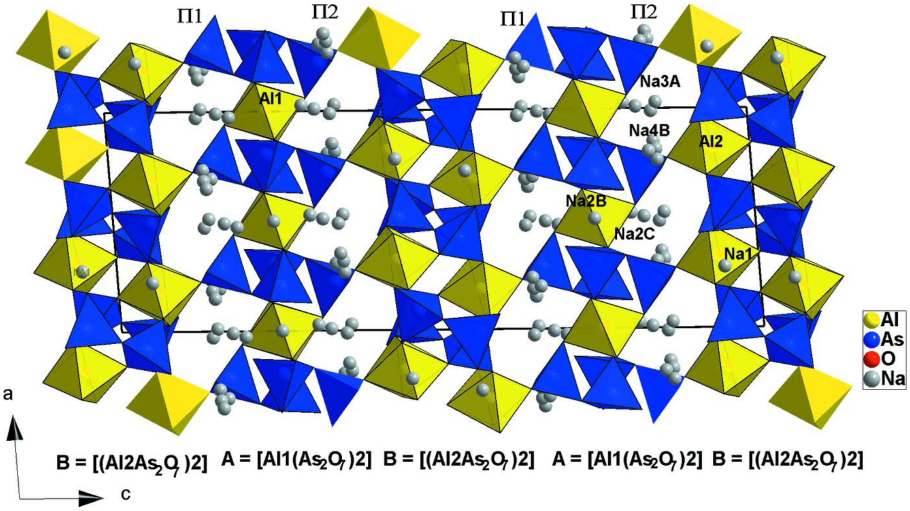

Figure 2

Projection of $Na_7Al_3(As_2O_7)_4$ structure along [010]. The Na sites are numbered. The picture indicates the location of the A and B layers and the π planes at $z \simeq 0.15$ and 0.35.

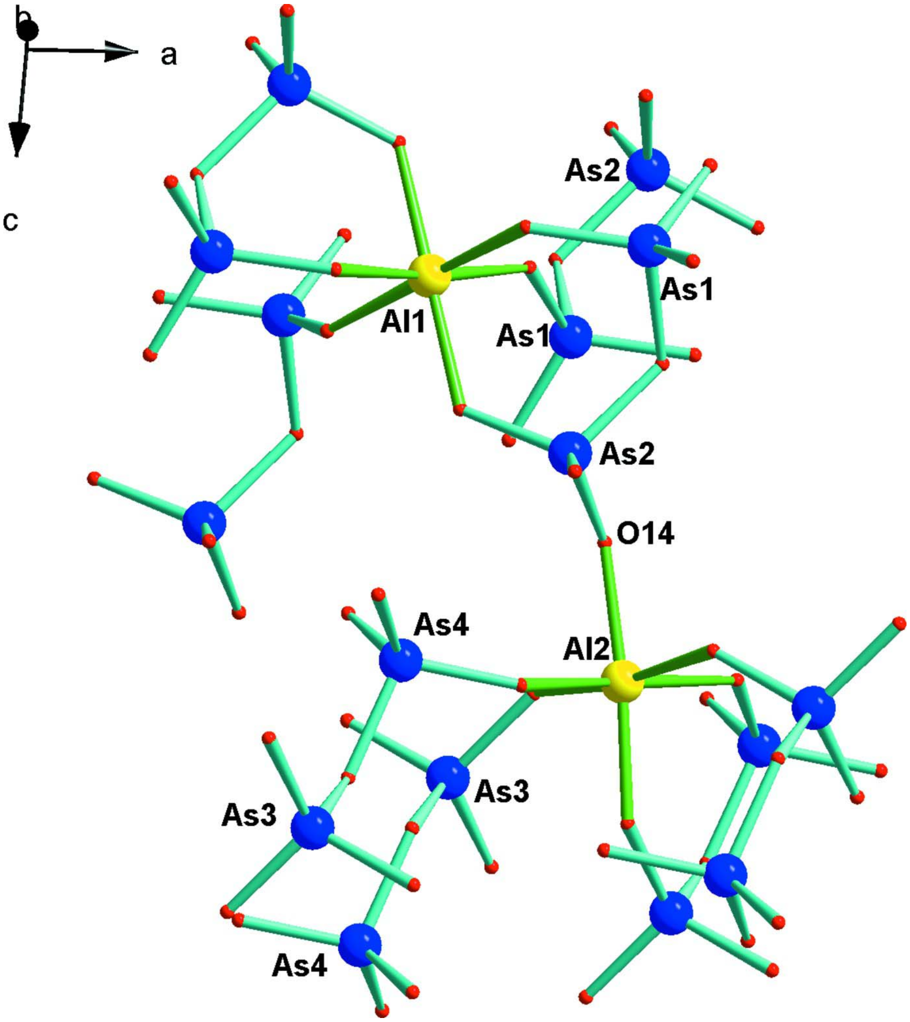

Figure 3

Arrangement of Al1O$_6$ octahedra and As1As2O$_7$ groups in the A-layer and arrangement of Al2O$_6$ octahedra and As3As4O$_7$ groups in the B-layer.

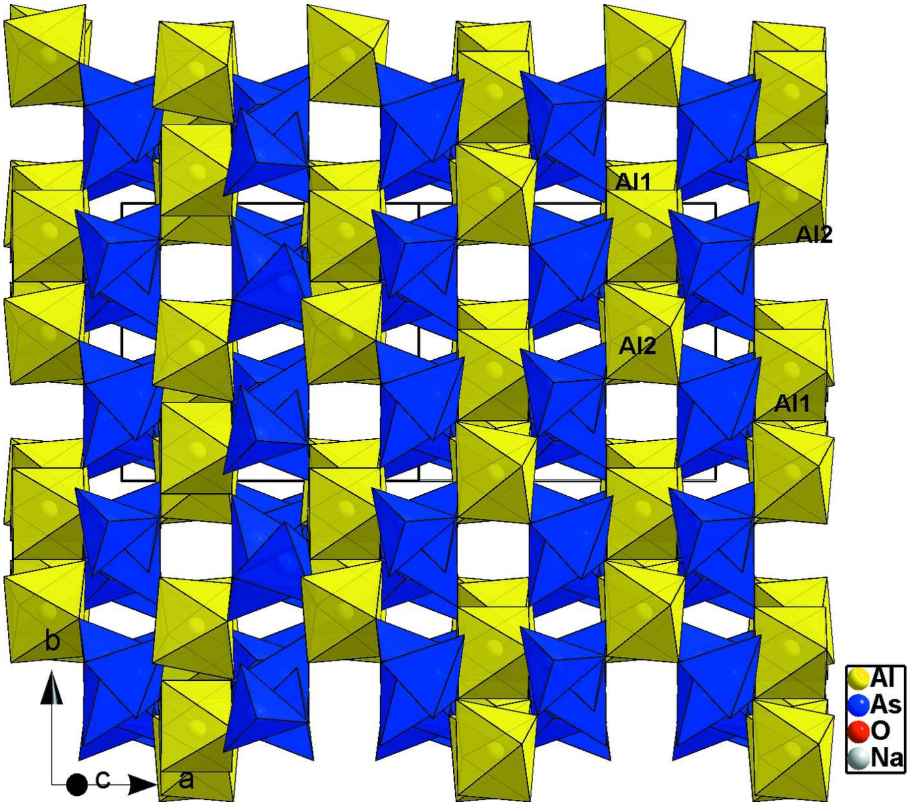

Figure 4

Alternate stacking of octahedral AlO_6 layers and As_2O_7 groups layers parallel to (-101).

Heptasodium trialuminium tetrakis(diarsenate)

Crystal data

$Na_7Al_3(As_2O_7)_4$
$M_r = 1289.23$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 9.800$ (1) Å
$b = 8.468$ (1) Å
$c = 28.637$ (2) Å
$\beta = 94.14$ (1)°
$V = 2370.3$ (4) Å^3
$Z = 4$
$F(000) = 2416$
$D_x = 3.613$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10–15°$
$\mu = 11.50$ mm^{-1}
$T = 298$ K
Parallelipiped, colorless
0.25 × 0.20 × 0.1 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)
$T_{min} = 0.759$, $T_{max} = 0.891$
3958 measured reflections
2583 independent reflections
2150 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.9°$
$h = -12 \rightarrow 3$
$k = -1 \rightarrow 10$
$l = -36 \rightarrow 36$
2 standard reflections every 120 min
intensity decay: 1.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.085$
$S = 1.10$
2583 reflections
221 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 24.9095P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.27$ e Å^{-3}
$\Delta\rho_{min} = -0.98$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00057 (6)

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)
Al1	0.0000	0.1057 (3)	0.2500	0.0082 (4)	
Al2	0.31736 (15)	−0.02622 (18)	0.43636 (5)	0.0069 (3)	
As1	0.30056 (5)	0.28137 (6)	0.246216 (18)	0.00898 (15)	
As2	0.21753 (5)	0.15080 (6)	0.338657 (18)	0.00927 (15)	
As3	0.58680 (5)	0.20071 (6)	0.464306 (18)	0.00733 (14)	
As4	0.48861 (5)	0.34009 (6)	0.557696 (18)	0.00774 (14)	
O1	0.3645 (4)	0.4537 (5)	0.26651 (14)	0.0149 (8)	
O2	0.3734 (4)	0.2071 (5)	0.20087 (13)	0.0149 (8)	
O3	0.1281 (4)	0.2823 (5)	0.23865 (14)	0.0148 (8)	
O4	0.3327 (4)	0.1491 (4)	0.29386 (13)	0.0119 (8)	
O5	0.4404 (4)	0.1537 (5)	0.43395 (15)	0.0170 (9)	
O6	0.6943 (4)	0.2857 (5)	0.42888 (14)	0.0145 (8)	
O7	0.6569 (4)	0.0529 (4)	0.49622 (13)	0.0120 (8)	
O8	0.5686 (4)	0.4760 (5)	0.59037 (13)	0.0148 (8)	
O9	0.3192 (4)	0.3690 (5)	0.54893 (14)	0.0142 (8)	
O10	0.5262 (4)	0.1554 (4)	0.57538 (14)	0.0133 (8)	
O11	0.5459 (4)	0.3542 (4)	0.50101 (13)	0.0139 (8)	
O12	0.0599 (4)	0.1063 (5)	0.31482 (14)	0.0162 (8)	
O13	0.2283 (5)	0.3289 (5)	0.36098 (15)	0.0210 (9)	
O14	0.2752 (4)	−0.0052 (5)	0.37014 (13)	0.0162 (8)	
Na1	−0.2221 (3)	−0.1225 (3)	0.44633 (9)	0.0249 (6)	
Na2A	0.5268 (10)	−0.0466 (12)	0.3075 (4)	0.017 (2)*	0.24
Na2B	0.5000	0.0010 (13)	0.2500	0.013 (2)*	0.28
Na2C	0.5094 (8)	−0.0556 (10)	0.3269 (3)	0.0236 (18)*	0.32
Na3A	0.0283 (5)	−0.1551 (6)	0.35860 (17)	0.0186 (11)*	0.58

Na3B	−0.0112 (8)	−0.1372 (9)	0.3504 (3)	0.0118 (16)*	0.33
Na4A	−0.233 (2)	0.100 (3)	0.3543 (7)	0.016 (4)*	0.13
Na4B	−0.1483 (11)	0.2292 (14)	0.3505 (3)	0.024 (2)*	0.27
Na4C	−0.1939 (9)	0.0862 (10)	0.3420 (3)	0.0220 (17)*	0.35
Na4D	−0.184 (2)	0.175 (3)	0.3538 (7)	0.025 (4)*	0.14

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0067 (9)	0.0083 (10)	0.0094 (10)	0.000	0.0000 (8)	0.000
Al2	0.0071 (7)	0.0064 (7)	0.0072 (7)	0.0000 (6)	−0.0004 (5)	0.0007 (6)
As1	0.0065 (2)	0.0108 (3)	0.0096 (3)	−0.00147 (19)	0.00072 (18)	0.00172 (19)
As2	0.0100 (3)	0.0103 (3)	0.0074 (3)	−0.0014 (2)	0.00003 (18)	0.0014 (2)
As3	0.0066 (2)	0.0081 (3)	0.0074 (3)	0.00032 (19)	0.00102 (18)	0.00067 (19)
As4	0.0076 (2)	0.0075 (3)	0.0083 (3)	−0.00002 (19)	0.00122 (18)	−0.00046 (18)
O1	0.0154 (19)	0.0102 (19)	0.019 (2)	−0.0034 (16)	0.0032 (15)	−0.0008 (16)
O2	0.0134 (18)	0.017 (2)	0.0151 (19)	−0.0001 (16)	0.0077 (14)	−0.0027 (16)
O3	0.0036 (16)	0.016 (2)	0.025 (2)	−0.0003 (15)	0.0023 (14)	0.0049 (17)
O4	0.0077 (16)	0.0145 (19)	0.0136 (18)	0.0026 (15)	0.0024 (14)	0.0037 (15)
O5	0.0125 (18)	0.0120 (19)	0.025 (2)	−0.0018 (15)	−0.0103 (16)	−0.0004 (16)
O6	0.0127 (18)	0.017 (2)	0.0149 (19)	0.0003 (16)	0.0066 (14)	0.0055 (16)
O7	0.0139 (18)	0.0114 (19)	0.0103 (18)	0.0063 (15)	−0.0011 (14)	0.0018 (15)
O8	0.0169 (19)	0.0147 (19)	0.013 (2)	−0.0044 (16)	0.0005 (15)	−0.0055 (15)
O9	0.0089 (17)	0.0145 (19)	0.019 (2)	0.0014 (15)	0.0009 (15)	0.0017 (16)
O10	0.0145 (18)	0.0076 (18)	0.018 (2)	0.0010 (15)	0.0025 (15)	0.0047 (15)
O11	0.025 (2)	0.0084 (18)	0.0088 (18)	0.0017 (16)	0.0077 (15)	0.0018 (15)
O12	0.0063 (16)	0.024 (2)	0.018 (2)	−0.0019 (16)	−0.0012 (14)	0.0011 (17)
O13	0.035 (2)	0.0112 (19)	0.017 (2)	−0.0013 (18)	0.0032 (17)	−0.0012 (17)
O14	0.022 (2)	0.0135 (19)	0.013 (2)	−0.0012 (16)	−0.0021 (15)	0.0030 (16)
Na1	0.0255 (13)	0.0141 (12)	0.0370 (15)	−0.0030 (10)	0.0148 (11)	−0.0035 (11)

Geometric parameters (Å, º)

Al1—O12^{i}	1.906 (4)	Na2B—O3^{ix}	2.274 (10)
Al1—O12	1.906 (4)	Na2B—O3^{iii}	2.274 (10)
Al1—O1^{ii}	1.932 (4)	Na2B—O4^{viii}	2.477 (7)
Al1—O1^{iii}	1.932 (4)	Na2B—O2^{viii}	2.512 (9)
Al1—O3	1.994 (4)	Na2C—O13^{ix}	2.492 (9)
Al1—O3^{i}	1.994 (4)	Na2C—O3^{iii}	2.619 (9)
Al2—O14	1.920 (4)	Na2C—O2^{viii}	2.652 (10)
Al2—O10^{iv}	1.933 (4)	Na2C—O12^{ix}	2.931 (9)
Al2—O7^{iv}	1.942 (4)	Na2C—O10^{iv}	2.968 (11)
Al2—O5	1.947 (4)	Na3A—O2^{iii}	2.330 (6)
Al2—O9^{v}	1.955 (4)	Na3A—O8^{v}	2.353 (6)
Al2—O6^{ii}	2.000 (4)	Na3A—O6^{ii}	2.545 (7)
As1—O2	1.651 (4)	Na3A—O5^{ii}	2.879 (6)
As1—O1	1.676 (4)	Na3A—O13^{ii}	2.949 (7)
As1—O3	1.689 (4)	Na3B—O8^{v}	2.279 (8)

As1—O4	1.776 (4)	Na3B—O2^{iii}	2.451 (8)
As2—O13	1.638 (4)	Na3B—O13^{ii}	2.608 (9)
As2—O14	1.675 (4)	Na3B—O1^{ii}	2.725 (9)
As2—O12	1.686 (4)	Na3B—O4^{ii}	2.807 (8)
As2—O4	1.769 (4)	Na3B—O6^{ii}	2.980 (9)
As3—O7	1.668 (4)	Na4A—O2^{i}	2.213 (19)
As3—O5	1.671 (4)	Na4A—O8^{v}	2.271 (19)
As3—O6	1.677 (4)	Na4A—O13^{ii}	2.33 (2)
As3—O11	1.736 (4)	Na4A—O6^{vii}	2.79 (2)
As4—O8	1.646 (4)	Na4B—O14^{x}	2.449 (11)
As4—O10	1.676 (4)	Na4B—O8^{v}	2.512 (11)
As4—O9	1.679 (4)	Na4B—O10^{v}	2.555 (11)
As4—O11	1.760 (4)	Na4B—O2^{i}	2.568 (11)
Na1—O8^{v}	2.265 (5)	Na4B—O3^{i}	2.613 (11)
Na1—O9^{vi}	2.302 (5)	Na4B—O6^{vii}	2.854 (11)
Na1—O7^{vii}	2.429 (4)	Na4C—O8^{v}	2.278 (8)
Na1—O13^{ii}	2.492 (5)	Na4C—O2^{i}	2.310 (9)
Na1—O5^{ii}	2.517 (5)	Na4C—O13^{ii}	2.384 (9)
Na1—O9^{ii}	2.938 (5)	Na4C—O1^{ii}	2.538 (10)
Na1—O11^{ii}	2.966 (5)	Na4C—O3^{i}	2.954 (9)
Na1—O10^{vi}	3.013 (5)	Na4D—O8^{v}	2.28 (2)
Na2A—O2^{viii}	2.380 (11)	Na4D—O2^{i}	2.36 (2)
Na2A—O3^{iii}	2.420 (10)	Na4D—O6^{vii}	2.70 (2)
Na2A—O13^{ix}	2.631 (11)	Na4D—O14^{x}	2.78 (3)
Na2A—O3^{ix}	2.692 (12)	Na4D—O10^{v}	2.85 (2)
Na2A—O12^{ix}	2.962 (11)	Na4D—O3^{i}	2.89 (2)

O12^{i}—Al1—O12	179.7 (3)	O2—As1—O4	107.54 (19)
O12^{i}—Al1—O1^{ii}	94.10 (18)	O1—As1—O4	103.99 (19)
O12—Al1—O1^{ii}	86.13 (17)	O3—As1—O4	102.82 (18)
O12^{i}—Al1—O1^{iii}	86.13 (17)	O13—As2—O14	120.4 (2)
O12—Al1—O1^{iii}	94.10 (18)	O13—As2—O12	113.3 (2)
O1^{ii}—Al1—O1^{iii}	96.5 (3)	O14—As2—O12	107.8 (2)
O12^{i}—Al1—O3	89.56 (18)	O13—As2—O4	105.3 (2)
O12—Al1—O3	90.19 (17)	O14—As2—O4	100.13 (19)
O1^{ii}—Al1—O3	172.35 (19)	O12—As2—O4	108.58 (18)
O1^{iii}—Al1—O3	90.44 (16)	O7—As3—O5	114.24 (19)
O12^{i}—Al1—O3^{i}	90.19 (17)	O7—As3—O6	113.67 (19)
O12—Al1—O3^{i}	89.56 (18)	O5—As3—O6	109.9 (2)
O1^{ii}—Al1—O3^{i}	90.44 (16)	O7—As3—O11	109.49 (18)
O1^{iii}—Al1—O3^{i}	172.35 (19)	O5—As3—O11	105.4 (2)
O3—Al1—O3^{i}	82.8 (2)	O6—As3—O11	103.15 (19)
O14—Al2—O10^{iv}	89.86 (18)	O8—As4—O10	113.3 (2)
O14—Al2—O7^{iv}	174.86 (18)	O8—As4—O9	114.1 (2)
O10^{iv}—Al2—O7^{iv}	93.40 (17)	O10—As4—O9	111.99 (19)
O14—Al2—O5	88.99 (18)	O8—As4—O11	107.83 (19)
O10^{iv}—Al2—O5	86.32 (18)	O10—As4—O11	105.32 (18)
O7^{iv}—Al2—O5	95.18 (18)	O9—As4—O11	103.31 (19)

O14—Al2—O9^{v}	92.74 (18)	As1—O1—Al1^{xi}	137.9 (2)
O10^{iv}—Al2—O9^{v}	170.74 (18)	As1—O3—Al1	127.7 (2)
O7^{iv}—Al2—O9^{v}	84.66 (17)	As2—O4—As1	117.7 (2)
O5—Al2—O9^{v}	84.85 (18)	As3—O5—Al2	132.7 (2)
O14—Al2—O6^{ii}	83.26 (17)	As3—O6—Al2^{xi}	132.6 (2)
O10^{iv}—Al2—O6^{ii}	90.59 (17)	As3—O7—Al2^{iv}	130.6 (2)
O7^{iv}—Al2—O6^{ii}	92.73 (17)	As4—O9—Al2^{v}	138.8 (2)
O5—Al2—O6^{ii}	171.67 (19)	As4—O10—Al2^{iv}	129.4 (2)
O9^{v}—Al2—O6^{ii}	98.54 (17)	As3—O11—As4	127.6 (2)
O2—As1—O1	115.63 (19)	As2—O12—Al1	127.1 (2)
O2—As1—O3	112.7 (2)	As2—O14—Al2	130.2 (2)
O1—As1—O3	112.73 (19)		

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