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NaSr(AsO₄)(H₂O)₉: the (Sr,As) analogue of nabaphite and nastrophite

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Key indicators: single-crystal X-ray study; T = 296 K; mean $\sigma(Na=O) = 0.0012$ Å; disorder in main residue; R factor = 0.023; wR factor = 0.056; data-to-parameter ratio = 57.2.

The crystal structure of the title compound, sodium strontium orthoarsenate(V) nonahydrate, is isotypic with NaSr(PO₄)-(H₂O)₉ and the minerals nabaphite [NaBa(PO₄)(H₂O)₉] and nastrophite [Na(Sr,Ba)(PO₄)(H₂O)₉]. The Na and Sr atoms are located on threefold rotation axes and are in the centres of slightly distorted Na(H₂O)₆ octahedra and Sr(H₂O)₉ tricapped trigonal prisms, respectively. A framework structure is established *via* edge-sharing of these polyhedra. Disordered AsO₄ tetrahedra (with threefold symmetry) are situated in the interstitial space of the framework. Although reasonable Hatom positions of the water molecules were not established, close O··O contacts between the disordered AsO₄ tetrahedra and the water molecules suggest strong O—H···O hydrogen bonding.

Related literature

For a previous study of the title compound that revealed cubic symmetry and the lattice parameters, see: Ariguib-Kbir & Guerin (1973). Isotypic structures have been reported for synthetic NaSr(PO₄)(H₂O)₉ (Takagi *et al.*, 1982), nabaphite [NaBa(PO₄)(H₂O)₉] (Baturin *et al.*, 1982) and nastrophite [Na(Sr,Ba)(PO₄)(H₂O)₉] (Baturin *et al.*, 1981). For crystal structures in the Sr-As-O-(H) system, see: Mihajlovic & Effenberger (2006); Weil *et al.* (2009). As-O bond-length data for tetrahedrally coordinated arsenic were compiled and computed by Baur (1981) and Schwendtner (2008). For ionic radii, see: Shannon (1976).

Experimental

Crystal data

NaSr(AsO₄)(H₂O)₉ $M_r = 411.67$ Cubic, $P2_13$ a = 10.6435 (1) Å V = 1205.74 (2) Å³ Z = 4 Mo $K\alpha$ radiation μ = 7.29 mm⁻¹ T = 296 K $0.36 \times 0.24 \times 0.24$ mm Data collection

Bruker APEXII CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2008) $T_{\min} = 0.179$, $T_{\max} = 0.274$ 41355 measured reflections 3435 independent reflections 3272 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.037$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$ $wR(F^2) = 0.056$ S = 1.073435 reflections 60 parameters $\Delta \rho_{\rm max} = 1.73 \ {\rm e} \ {\rm \mathring{A}}^{-3}$ $\Delta \rho_{\rm min} = -1.66 \ {\rm e} \ {\rm \mathring{A}}^{-3}$ Absolute structure: Flack (1983), 1537 Friedel pairs Flack parameter: -0.005 (6)

H-atom parameters not refined

 Table 1

 Selected interatomic distances (Å).

Sr-O1 ⁱ	2.6326 (10)	Na-O3 ⁱⁱⁱ	2.3926 (12)
Sr-O2	2.6558 (10)	$Na - O2^{iv}$	2.4086 (12)
Sr-O3 ⁱⁱ	2.6994 (10)		
$O1 \cdot \cdot \cdot O5^v$	2.558 (7)	O2···O6 ^{vii}	2.7488 (17)
O1···O5	2.612 (8)	$O3 \cdots O8^{vi}$	2.562 (9)
$O1 \cdot \cdot \cdot O9^{vi}$	2.623 (8)	$O3 \cdot \cdot \cdot O6^{vi}$	2.6949 (17)
O1···O6 ^{vii}	2.6640 (17)	$O3 \cdot \cdot \cdot O9^{vi}$	2.732 (9)
O1···O4	2.7667 (14)	O3···O6	2.7492 (17)
O1···O7	2.829 (5)	O3···O5	2.757 (7)
$O1 \cdot \cdot \cdot O7^{vi}$	2.919 (5)	O3···O7	2.776 (5)
$O2 \cdot \cdot \cdot O9^{vi}$	2.515 (9)	$O3 \cdot \cdot \cdot O7^{vi}$	2.930 (5)

Symmetry codes: (i) $-x + \frac{1}{2}, -y, z - \frac{1}{2}$; (ii) $-z, x - \frac{1}{2}, -y + \frac{1}{2}$; (iii) $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$; (iv) $-z + \frac{1}{2}, -x + 1, y + \frac{1}{2}$; (v) y, z, x; (vi) $-z + 1, x - \frac{1}{2}, -y + \frac{1}{2}$; (vii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.

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: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS for Windows* (Dowty, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2248).

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NaSr(AsO₄)(H₂O)₉: the (Sr,As) analogue of nabaphite and nastrophite

Matthias Weil

S1. Comment

A previous study of NaSr(AsO₄)(H₂O)₉ reports cubic symmetry and the lattice parameter as a = 10.70 Å (Ariguib-Kbir & Guerin, 1973). Moreover, isotypism with NaSr(PO₄)(H₂O)₉ (Takagi *et al.*, 1982) was also revealed. Besides the synthetic phosphate analogue, NaSr(AsO₄)(H₂O)₉ is also isotypic with the minerals nabaphite [NaBa(PO₄)(H₂O)₉] (Baturin *et al.*, 1982) and nastrophite [Na(Sr,Ba)(PO₄)(H₂O)₉] (Baturin *et al.*, 1981).

The crystal structures consist of slightly distorted Na(OH₂)₆ octahedra (3 symmetry) and M(OH₂)₉ tricapped trigonal prisms (3 symmetry), where M = Sr, Ba. These polyhedra share edges and establish a framework structure. Disordered XO_4 tetrahedra (X = P, As; 3 symmetry) are situated in the interstitial space of the framework (Fig. 1).

The Na(H₂O)₆ octahedron is slightly distorted. The corresponding Na—O bond lengths are in the usual range with an average of 2.40 Å, conform with the values in the isotypic compounds (NaSr(PO₄)(H₂O)₉: 2.41 Å; nabaphite: 2.42 Å; nastrophite: 2.42 Å) and the sum of the ionic radii of 2.41 Å, as calculated for six-coordinated Na (Shannon, 1976).

The Sr²⁺ ion is surrounded by 9 oxygen atoms with an average Sr—O distance of 2.663 Å, in good agreement with the phosphate analogue (2.668 Å; Takagi *et al.*, 1982) and the sum of the ionic radii of 2.67 Å, as calculated for nine-coordinated Sr (Shannon, 1976).

The environment of the disordered AsO₄ group consists of 16 water molecules with donor (D) — acceptor (A) distances between 2.5 and 3.0 Å (see Table 2). The overcrowding of water molecules (only 12 surrounding O atoms are expected, considering an ordered tetrahedral configuration for the arsenate unit with three donator atoms) may be the reason for the disorder of the AsO₄ group. The average As—O bond length for the disordered AsO₄ group is 1.685 Å, a value in very good agreement with those of 1.682 Å (Baur, 1981) and 1.686 Å (Schwendtner, 2008).

S2. Experimental

Crystals of the title compound were obtained during phase formation studies in the system Sr—As—O (Weil *et al.*, 2009) from hydrous solutions. All chemicals used were of analytical grade and employed without further purification. To a saturated Sr(OH)₂·8H₂O solution a diluted arsenic acid solution was dropwise added which resulted in a flocculent white precipitate (pH *ca.* 9). A concentrated NaOH solution was then added until a pH of 12 was reached. The resulting suspension was boiled for an hour. Then the precipitate was filtered off and the remaining solution was left to stand for several days. Besides few crystals of SrHAsO₄ (Mihajlovic & Effenberger, 2006), colourless columnar crystals of the title compound up to several mm in length were obtained after complete evaporation of water.

S3. Refinement

The oxygen atoms O4 and O6 of the arsenate group were clearly discernible from Fourier maps. Consideration of full occupancy of these sites resulted in high electron densities of ca 4 e Å³ at a distance of ca 1.7 Å from As, indicating other disordered oxygen atoms. Therefore four additional O atoms were considered in the final model. Free refinement of the

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site occupancy factors (s.o.f.) of all six O atoms attached to arsenic resulted in a composition very close to the theoretical value. In the last refinement cycles the s.o.f.'s were constrained to meet the criterion for electroneutrality. The six disordered O atoms were finally refined with isotropic displacement parameters. No reasonable positions of the H atoms attached to the water molecules (O1, O2, O3) could be found in difference Fourier maps which may be due to the disorder of the AsO₄ tetrahedron and the resulting complex hydrogen bonding scheme. Therefore all H atoms were excluded from the refinement. The highest remaining peak in the final difference Fourier map is 0.49 Å from As and the deepest hole is 0.43 Å from the same atom.

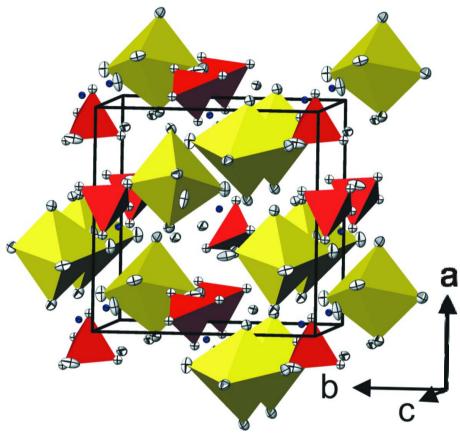


Figure 1

The crystal structure of $NaSr(PO_4)(H_2O)_9$ in a projection approximately along [001]. Sr atoms are represented as blue spheres and O atoms as white spheres; NaO_6 octahedra are given in yellow and AsO_4 tetrahedra in red. For clarity, Sr—O bonds are omitted and only one orientation of the disordered AsO_4 group is given. Ellipsoids are drawn at the 90% probability level.

sodium strontium orthoarsenate(V) nonahydrate

Crystal data

NaSr(AsO₄)(H₂O)₉ $M_r = 411.67$ Cubic, $P2_13$ Hall symbol: P 2ac 2ab 3 a = 10.6435 (1) Å V = 1205.74 (2) Å³ Z=4 F(000)=816 $D_{\rm x}=2.268~{\rm Mg~m^{-3}}$ Mo $K\alpha$ radiation, $\lambda=0.71073~{\rm Å}$ Cell parameters from 9782 reflections $\theta=5.8$ – 45.2° $\mu = 7.29 \text{ mm}^{-1}$ T = 296 K

Data collection

Bruker APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω and φ scans

Absorption correction: multi-scan (SADABS; Bruker, 2008)

 $T_{\min} = 0.179, T_{\max} = 0.274$

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.023$ $wR(F^2) = 0.056$

S = 1.07

3435 reflections

60 parameters 0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Fragment, colourless $0.36 \times 0.24 \times 0.24$ mm

41355 measured reflections 3435 independent reflections 3272 reflections with $I > 2\sigma(I)$

 $R_{\rm int}=0.037$

 $\theta_{\text{max}} = 45.7^{\circ}, \ \theta_{\text{min}} = 5.4^{\circ}$

 $h = -21 \rightarrow 21$

 $k = -20 \rightarrow 21$

 $l = -17 \rightarrow 17$

H-atom parameters not refined

 $w = 1/[\sigma^2(F_0^2) + (0.0274P)^2 + 0.5628P]$

where $P = (F_0^2 + 2F_c^2)/3$

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

 $\Delta \rho_{\text{max}} = 1.73 \text{ e Å}^{-3}$

 $\Delta \rho_{\min} = -1.66 \text{ e Å}^{-3}$

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

Extinction coefficient: 0.0147 (10)

Absolute structure: Flack (1983), 1537 Friedel

pairs

Absolute structure parameter: -0.005 (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 F-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

	x	y	Z	$U_{ m iso}$ */ $U_{ m eq}$	Occ. (<1)
Sr	0.055001 (8)	0.055001 (8)	0.055001 (8)	0.00459(3)	
As	0.421839 (11)	0.421839 (11)	0.421839 (11)	0.00709 (4)	
Na	0.67077 (6)	0.67077 (6)	0.67077 (6)	0.01193 (15)	
O1	0.39368 (12)	0.07909 (10)	0.35359 (10)	0.01687 (18)	
O2	0.29270 (9)	0.13067 (11)	0.04892 (10)	0.01519 (16)	
О3	0.60854 (10)	0.29633 (9)	0.14338 (10)	0.01243 (14)	
O4	0.33000 (13)	0.33000 (13)	0.33000 (13)	0.0077 (3)*	0.60
O5	0.4046 (7)	0.3186 (7)	0.3016 (7)	0.0117 (10)*	0.13
O6	0.56151 (12)	0.44234 (13)	0.35120 (12)	0.00759 (17)*	0.60
O7	0.5256 (5)	0.3069 (5)	0.3904 (5)	0.0115 (7)*	0.20
O8	0.5623 (8)	0.3833 (8)	0.4407 (8)	0.0088 (11)*	0.10
O9	0.5627 (8)	0.3668 (8)	0.4973 (8)	0.0084 (11)*	0.10

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Atomic displacement parameters (\mathring{A}^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr	0.00459(3)	0.00459(3)	0.00459(3)	0.00016 (2)	0.00016 (2)	0.00016 (2)
As	0.00709 (4)	0.00709 (4)	0.00709 (4)	-0.00024(3)	-0.00024(3)	-0.00024(3)
Na	0.01193 (15)	0.01193 (15)	0.01193 (15)	0.00126 (17)	0.00126 (17)	0.00126 (17)
O1	0.0319 (5)	0.0088(3)	0.0098(3)	0.0043 (3)	-0.0045(3)	-0.0005(3)
O2	0.0109(3)	0.0229 (4)	0.0118 (3)	-0.0039(3)	0.0002(3)	0.0007 (3)
O3	0.0130(3)	0.0111 (3)	0.0132 (3)	0.0024(3)	-0.0005 (3)	0.0015 (3)

Geometric parameters (Å, °)					
Sr—O1 ⁱ	2.6326 (10)	As—O9iv	1.799 (9)		
Sr—O1 ⁱⁱ	2.6326 (10)	$As-O9^{v}$	1.799 (9)		
Sr—O1 ⁱⁱⁱ	2.6326 (10)	Na—O3 ^{ix}	2.3926 (12)		
Sr — $O2^{iv}$	2.6558 (10)	Na—O3 ^x	2.3926 (12)		
Sr—O2	2.6558 (10)	Na—O3 ^{xi}	2.3926 (12)		
Sr—O2 ^v	2.6558 (10)	Na—O2 ^{xii}	2.4086 (12)		
Sr — $O3^{vi}$	2.6994 (10)	Na—O2xiii	2.4086 (12)		
Sr—O3vii	2.6994 (10)	Na—O2 ^{xiv}	2.4086 (12)		
Sr—O3viii	2.6994 (10)	$O4$ — $O5^{iv}$	0.858 (7)		
As — $O8^{iv}$	1.563 (8)	O4—O5	0.858 (7)		
As—O8	1.563 (8)	O4—O5 ^v	0.858 (7)		
As—O8 ^v	1.563 (8)	O5—O5 ^v	1.440 (13)		
As—O6	1.6801 (13)	$O5$ — $O5^{iv}$	1.440 (13)		
$As-O6^{\circ}$	1.6801 (13)	O5—O7	1.602 (9)		
As — $O6^{iv}$	1.6801 (13)	O6—O8	1.141 (9)		
$As-O7^{iv}$	1.682 (5)	O6—O9 ^v	1.462 (9)		
As—O7	1.682 (5)	O6—O7	1.549 (5)		
As—O7°	1.682 (5)	O6—O9	1.750 (8)		
As—O4	1.693 (2)	O7—O8	1.049 (10)		
As — $O5^{iv}$	1.697 (7)	O7—O9	1.362 (9)		
As—O5	1.697 (7)	O8—O9	0.627 (11)		
As—O5°	1.697 (7)	$O9$ — $O6^{iv}$	1.462 (9)		
As—O9	1.799 (9)				
O1···O5 ^{iv}	2.558 (7)	O2···O6 ^{xvi}	2.7488 (17)		
O1···O5	2.612 (8)	$O3\cdots O8^{xv}$	2.562 (9)		
O1…O9xv	2.623 (8)	$O3\cdots O6^{xv}$	2.6949 (17)		
$O1\cdots O6^{xvi}$	2.6640 (17)	$O3\cdots O9^{xv}$	2.732 (9)		
O1···O4	2.7667 (14)	O3···O6	2.7492 (17)		
O1···O7	2.829 (5)	O3···O5	2.757 (7)		
O1···O7 ^{xv}	2.919 (5)	O3···O7	2.776 (5)		
O2···O9 ^{xv}	2.515 (9)	O3···O7 ^{xv}	2.930 (5)		
O1 ⁱ —Sr—O1 ⁱⁱ	80.79 (4)	$O8^v$ — As — $O5^{iv}$	140.9 (4)		
$O1^{i}$ — Sr — $O1^{iii}$	80.79 (4)	$O6$ — As — $O5^{iv}$	128.5 (3)		
O1 ⁱⁱ —Sr—O1 ⁱⁱⁱ	80.79 (4)	$O6^v$ — As — $O5^{iv}$	113.1 (3)		

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$O1^{i}$ — Sr — $O2^{iv}$	86.96 (4)	$O6^{iv}$ — As — $O5^{iv}$	80.9 (3)
$O1^{ii}$ — Sr — $O2^{iv}$	134.39 (3)	$O7^{iv}$ —As— $O5^{iv}$	56.6 (3)
$O1^{iii}$ — Sr — $O2^{iv}$	140.21 (3)	$O7$ — As — $O5^{iv}$	81.6 (3)
O1 ⁱ —Sr—O2	140.21 (3)	$O7^{v}$ — As — $O5^{iv}$	106.7 (3)
O1 ⁱⁱ —Sr—O2	86.96 (4)	O8iv—As—O5	140.9 (4)
O1 ⁱⁱⁱ —Sr—O2	134.39 (3)	O8—As—O5	91.7 (4)
$O2^{iv}$ — Sr — $O2$	75.03 (4)	O8 ^v —As—O5	115.8 (4)
O1 ⁱ —Sr—O2 ^v	134.39 (3)	O6—As—O5	80.9 (3)
$O1^{ii}$ — Sr — $O2^{v}$	140.21 (3)	O6 ^v —As—O5	128.5 (3)
O1 ⁱⁱⁱ —Sr—O2 ^v	86.96 (4)	$O6^{iv}$ —As— $O5$	113.1 (3)
$O2^{iv}$ — Sr — $O2^{v}$	75.03 (4)	O7 ^{iv} —As—O5	106.7 (3)
O2—Sr—O2 ^v	75.03 (4)	O7—As—O5	56.6 (3)
$O1^{i}$ — Sr — $O3^{vi}$	68.72 (3)	O7 ^v —As—O5	81.6 (3)
$O1^{ii}$ — Sr — $O3^{vi}$	68.05 (3)	$O5^{iv}$ —As— $O5$	50.2 (4)
O1 ⁱⁱⁱ —Sr—O3 ^{vi}	138.94 (4)	$O8^{iv}$ — As — $O9$	80.4 (4)
$O2^{iv}$ — Sr — $O3^{vi}$	66.55 (3)	O8v—As—O9	108.7 (4)
O2—Sr—O3 ^{vi}	71.58 (3)	O8—As—O9	19.9 (4)
$O2^{v}$ — Sr — $O3^{vi}$	134.06 (3)	O6 ^v —As—O9	127.1 (3)
O1 ⁱ —Sr—O3 ^{vii}	68.05 (3)	O6—As—O9	60.3 (3)
$O1^{ii}$ — Sr — $O3^{vii}$	138.94 (4)	O6 ^{iv} —As—O9	49.6 (3)
O1 ⁱⁱⁱ —Sr—O3 ^{vii}	68.72 (3)	O7 ^{iv} —As—O9	104.4 (3)
$O2^{iv}$ — Sr — $O3^{vii}$	71.58 (3)	O7—As—O9	45.9 (3)
O2—Sr—O3 ^{vii}	134.06 (3)	O7 ^v —As—O9	134.8 (3)
$O2^{v}$ — Sr — $O3^{vii}$	66.55 (3)	O4—As—O9	123.4 (3)
$O3^{vi}$ — Sr — $O3^{vii}$	119.992 (1)	$O5^{iv}$ —As— $O9$	110.0 (4)
O1 ⁱ —Sr—O3 ^{viii}	138.94 (4)	O5—As—O9	102.5 (4)
O1 ⁱⁱ —Sr—O3 ^{viii}	68.72 (3)	O5 ^v —As—O9	152.0 (4)
O1 ⁱⁱⁱ —Sr—O3 ^{viii}	68.05 (3)	$O8^{iv}$ — As — $O9^{iv}$	19.9 (4)
$O2^{iv}$ — Sr — $O3^{viii}$	134.06 (3)	$O8^{v}$ — As — $O9^{iv}$	80.4 (4)
O2—Sr—O3 ^{viii}	66.55 (3)	$O8$ — As — $O9^{iv}$	108.7 (4)
O2 ^v —Sr—O3 ^{viii}	71.58 (3)	$O6^v$ — As — $O9^{iv}$	49.6 (3)
$O3^{vi}$ — Sr — $O3^{viii}$	119.992 (1)	O6—As—O9iv	127.1 (3)
O3 ^{vii} —Sr—O3 ^{viii}	119.992 (1)	$O6^{iv}$ — As — $O9^{iv}$	60.3 (3)
$O8^{iv}$ — As — $O8$	99.3 (4)	$O7^{iv}$ —As— $O9^{iv}$	45.9 (3)
$O8^{iv}$ — As — $O8^{v}$	99.3 (4)	O7—As—O9 ^{iv}	134.8 (3)
O8—As—O8 ^v	99.3 (4)	O7 ^v —As—O9 ^{iv}	104.4 (3)
O8 ^{iv} —As—O6	130.1 (3)	O4—As—O9 ^{iv}	123.4 (3)
O8 ^v —As—O6	69.2 (3)	$O5^{iv}$ — As — $O9^{iv}$	102.5 (4)
$O8^{iv}$ — As — $O6^{v}$	69.2 (3)	O5—As—O9iv	152.0 (4)
O8—As—O6°	130.1 (3)	O5 ^v —As—O9 ^{iv}	110.0 (4)
O6—As—O6 ^v	109.83 (4)	O9—As—O9 ^{iv}	92.6 (4)
$O8$ — As — $O6^{iv}$	69.2 (3)	$O8^{iv}$ — As — $O9^{v}$	108.7 (4)
$O8^{v}$ — As — $O6^{iv}$	130.1 (3)	$O8^{v}$ — As — $O9^{v}$	19.9 (4)
$O6$ — As — $O6^{iv}$	109.83 (4)	O8—As—O9 ^v	80.4 (4)
$O6^{v}$ — As — $O6^{iv}$	109.83 (4)	$O6^{v}$ — As — $O9^{v}$	60.3 (3)
O8—As—O7 ^{iv}	124.0 (4)	O6—As—O9 ^v	49.6 (3)
$O8^{v}$ — As — $O7^{iv}$	117.1 (3)	$O6^{iv}$ — As — $O9^v$	127.1 (3)
O6—As—O7 ^{iv}	164.45 (18)	O7 ^{iv} —As—O9 ^v	134.8 (3)

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supporting information

$O6^{v}$ —As— $O7^{iv}$	76.41 (17)	O7—As—O9 ^v	104.4 (3)
$O6^{iv}$ — As — $O7^{iv}$	54.87 (18)	O7 ^v —As—O9 ^v	45.9 (3)
$O8^{iv}$ — As — $O7$	117.1 (3)	O4—As—O9 ^v	123.4 (3)
O8°—As—O7	124.0 (4)	$O5^{iv}$ —As— $O9^{v}$	152.0 (4)
O6—As—O7	54.87 (18)	O5—As—O9 ^v	110.0 (4)
O6°—As—O7	164.45 (18)	$O5^{v}$ — As — $O9^{v}$	102.5 (4)
$O6^{iv}$ —As— $O7$	76.41 (17)	O9—As—O9 ^v	92.6 (4)
$O7^{iv}$ —As— $O7$	117.62 (9)	$O9^{iv}$ — As — $O9^{v}$	92.6 (4)
$O8^{iv}$ — As — $O7^{v}$	124.0 (4)	$O3^{ix}$ — Na — $O3^x$	89.64 (5)
O8—As—O7 ^v	117.1 (3)	$O3^{ix}$ — Na — $O3^{xi}$	89.65 (5)
O6—As—O7 ^v	76.41 (17)	$O3^{x}$ — Na — $O3^{xi}$	89.64 (5)
O6°—As—O7°	54.87 (18)	$O3^{ix}$ —Na— $O2^{xii}$	75.47 (4)
$O6^{iv}$ — As — $O7^v$	164.45 (18)	O3 ^x —Na—O2 ^{xii}	155.21 (3)
$O7^{iv}$ —As— $O7^{v}$	117.62 (9)	$O3^{xi}$ — Na — $O2^{xii}$	109.62 (4)
O7—As—O7 ^v	117.62 (9)	O3 ^{ix} —Na—O2 ^{xiii}	109.62 (4)
$O8^{iv}$ — As — $O4$	118.4 (3)	O3 ^x —Na—O2 ^{xiii}	75.47 (4)
O8—As—O4	118.4 (3)	$O3^{xi}$ —Na— $O2^{xiii}$	155.21 (3)
O8 ^v —As—O4	118.4 (3)	O2 ^{xii} —Na—O2 ^{xiii}	90.76 (5)
O6—As—O4	109.11 (5)	$O3^{ix}$ — Na — $O2^{xiv}$	155.21 (3)
O6°—As—O4	109.11 (5)	$O3^{x}$ — Na — $O2^{xiv}$	109.62 (4)
$O6^{iv}$ —As— $O4$	109.11 (5)	$O3^{xi}$ — Na — $O2^{xiv}$	75.47 (4)
$O7^{iv}$ —As— $O4$	81.04 (17)	$O2^{xii}$ —Na— $O2^{xiv}$	90.76 (5)
O7—As—O4	81.04 (17)	$O2^{xiii}$ — Na — $O2^{xiv}$	90.76 (5)
O7 ^v —As—O4	81.04 (17)	Na ^{xvi} —O2—Sr	103.37 (4)
$O8^{iv}$ — As — $O5^{iv}$	91.7 (4)	Na ^{xvii} —O3—Sr ^{xviii}	102.52 (4)
$O8$ — As — $O5^{iv}$	115.8 (4)		

 $\begin{array}{l} \text{Symmetry codes: } (i) -y, z - 1/2, -x + 1/2; \\ (ii) -x + 1/2, -y, z - 1/2; \\ (iii) z - 1/2, -x + 1/2, -y; \\ (iv) y - z, x; \\ (v) z, x, y; \\ (v) z,$

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