

## NaSr(AsO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>: the (Sr,As) analogue of nabaphite and nastrophite

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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{Na}–\text{O}) = 0.0012$  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(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub> and the minerals nabaphite [NaBa(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>] and nastrophite [Na(Sr,Ba)(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>]. The Na and Sr atoms are located on threefold rotation axes and are in the centres of slightly distorted Na(H<sub>2</sub>O)<sub>6</sub> octahedra and Sr(H<sub>2</sub>O)<sub>9</sub> tricapped trigonal prisms, respectively. A framework structure is established *via* edge-sharing of these polyhedra. Disordered AsO<sub>4</sub> tetrahedra (with threefold symmetry) are situated in the interstitial space of the framework. Although reasonable H-atom positions of the water molecules were not established, close O· · · O contacts between the disordered AsO<sub>4</sub> 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(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub> (Takagi *et al.*, 1982), nabaphite [NaBa(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>] (Baturin *et al.*, 1982) and nastrophite [Na(Sr,Ba)(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>] (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(AsO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>  
 $M_r = 411.67$   
Cubic,  $P2_13$   
 $a = 10.6435$  (1) Å  
 $V = 1205.74$  (2) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 7.29$  mm<sup>-1</sup>  
 $T = 296$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$   
 $wR(F^2) = 0.056$   
 $S = 1.07$   
3435 reflections  
60 parameters  
H-atom parameters not refined

$\Delta\rho_{\max} = 1.73$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.66$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
1537 Friedel pairs  
Flack parameter: -0.005 (6)

**Table 1**  
Selected interatomic distances (Å).

Sr–O1 <sup>i</sup>	2.6326 (10)	Na–O3 <sup>iii</sup>	2.3926 (12)
Sr–O2	2.6558 (10)	Na–O2 <sup>iv</sup>	2.4086 (12)
Sr–O3 <sup>ii</sup>	2.6994 (10)		
O1···O5 <sup>v</sup>	2.558 (7)	O2···O6 <sup>vii</sup>	2.7488 (17)
O1···O5	2.612 (8)	O3···O8 <sup>vi</sup>	2.562 (9)
O1···O9 <sup>vi</sup>	2.623 (8)	O3···O6 <sup>vi</sup>	2.6949 (17)
O1···O6 <sup>vii</sup>	2.6640 (17)	O3···O9 <sup>vi</sup>	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 <sup>vi</sup>	2.919 (5)	O3···O7	2.776 (5)
O2···O9 <sup>vi</sup>	2.515 (9)	O3···O7 <sup>vi</sup>	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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## **supplementary materials**

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## **NaSr(AsO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>: the (Sr,As) analogue of nabaphite and nastrophite**

**M. Weil**

### **Comment**

A previous study of NaSr(AsO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub> reports cubic symmetry and the lattice parameter as  $a = 10.70 \text{ \AA}$  (Arguib-Kbir & Guerin, 1973). Moreover, isoty whole with NaSr(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub> (Takagi *et al.*, 1982) was also revealed. Besides the synthetic phosphate analogue, NaSr(AsO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub> is also isotopic with the minerals nabaphite [NaBa(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>] (Baturin *et al.*, 1982) and nastrophite [Na(Sr,Ba)(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>] (Baturin *et al.*, 1981).

The crystal structures consist of slightly distorted Na(OH<sub>2</sub>)<sub>6</sub> octahedra (3 symmetry) and  $M(\text{OH}_2)_9$  tricapped trigonal prisms (3 symmetry), where  $M = \text{Sr, Ba}$ . These polyhedra share edges and establish a framework structure. Disordered  $X\text{O}_4$  tetrahedra ( $X = \text{P, As}$ ; 3 symmetry) are situated in the interstitial space of the framework (Fig. 1).

The Na(H<sub>2</sub>O)<sub>6</sub> 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 isotopic compounds (NaSr(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub>: 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 Sr<sup>2+</sup> 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 AsO<sub>4</sub> 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 donor atoms) may be the reason for the disorder of the AsO<sub>4</sub> group. The average As—O bond length for the disordered AsO<sub>4</sub> 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).

### **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)<sub>2</sub>·8H<sub>2</sub>O 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 SrHASO<sub>4</sub> (Mihajlovic & Effenberger, 2006), colourless columnar crystals of the title compound up to several mm in length were obtained after complete evaporation of water.

# supplementary materials

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## 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 Å<sup>3</sup> 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 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 AsO<sub>4</sub> 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.

## Figures

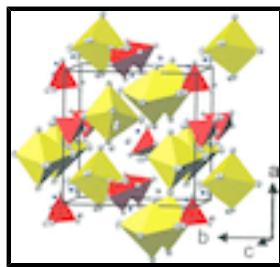


Fig. 1. The crystal structure of NaSr(PO<sub>4</sub>)(H<sub>2</sub>O)<sub>9</sub> in a projection approximately along [001]. Sr atoms are represented as blue spheres and O atoms as white spheres; NaO<sub>6</sub> octahedra are given in yellow and AsO<sub>4</sub> tetrahedra in red. For clarity, Sr—O bonds are omitted and only one orientation of the disordered AsO<sub>4</sub> group is given. Ellipsoids are drawn at the 90% probability level.

## sodium strontium orthoarsenate(V) nonahydrate

### Crystal data

NaSr(AsO <sub>4</sub> )(H <sub>2</sub> O) <sub>9</sub>	$Z = 4$
$M_r = 411.67$	$F_{000} = 816$
Cubic, $P\bar{2}_13$	$D_x = 2.268 \text{ Mg m}^{-3}$
Hall symbol: P 2ac 2ab 3	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 10.6435 (1) \text{ \AA}$	Cell parameters from 9782 reflections
$b = 10.6435 (1) \text{ \AA}$	$\theta = 5.8\text{--}45.2^\circ$
$c = 10.6435 (1) \text{ \AA}$	$\mu = 7.29 \text{ mm}^{-1}$
$\alpha = 90^\circ$	$T = 296 \text{ K}$
$\beta = 90^\circ$	Fragment, colourless
$\gamma = 90^\circ$	$0.36 \times 0.24 \times 0.24 \text{ mm}$
$V = 1205.74 (2) \text{ \AA}^3$	

### Data collection

Bruker APEXII CCD diffractometer	3435 independent reflections
Radiation source: fine-focus sealed tube	3272 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.037$

$T = 296 \text{ K}$	$\theta_{\max} = 45.7^\circ$
$\omega$ and $\varphi$ scans	$\theta_{\min} = 5.4^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2008)	$h = -21 \rightarrow 21$
$T_{\min} = 0.179$ , $T_{\max} = 0.274$	$k = -20 \rightarrow 21$
41355 measured reflections	$l = -17 \rightarrow 17$

### Refinement

Refinement on $F^2$	H-atom parameters not refined
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.5628P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$(\Delta/\sigma)_{\max} = 0.001$
$wR(F^2) = 0.056$	$\Delta\rho_{\max} = 1.73 \text{ e \AA}^{-3}$
$S = 1.07$	$\Delta\rho_{\min} = -1.66 \text{ e \AA}^{-3}$
3435 reflections	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{1/4}$
60 parameters	Extinction coefficient: 0.0147 (10)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1537 Friedel pairs
Secondary atom site location: difference Fourier map	Flack 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  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	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)	
O3	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

## supplementary materials

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O9	0.5627 (8)	0.3668 (8)	0.4973 (8)	0.0084 (11)*	0.10
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*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 ( $\text{\AA}$ ,  $^\circ$ )*

Sr—O1 <sup>i</sup>	2.6326 (10)	As—O9 <sup>iv</sup>	1.799 (9)
Sr—O1 <sup>ii</sup>	2.6326 (10)	As—O9 <sup>v</sup>	1.799 (9)
Sr—O1 <sup>iii</sup>	2.6326 (10)	Na—O3 <sup>ix</sup>	2.3926 (12)
Sr—O2 <sup>iv</sup>	2.6558 (10)	Na—O3 <sup>x</sup>	2.3926 (12)
Sr—O2	2.6558 (10)	Na—O3 <sup>xi</sup>	2.3926 (12)
Sr—O2 <sup>v</sup>	2.6558 (10)	Na—O2 <sup>xii</sup>	2.4086 (12)
Sr—O3 <sup>vi</sup>	2.6994 (10)	Na—O2 <sup>xiii</sup>	2.4086 (12)
Sr—O3 <sup>vii</sup>	2.6994 (10)	Na—O2 <sup>xiv</sup>	2.4086 (12)
Sr—O3 <sup>viii</sup>	2.6994 (10)	O4—O5 <sup>iv</sup>	0.858 (7)
As—O8 <sup>iv</sup>	1.563 (8)	O4—O5	0.858 (7)
As—O8	1.563 (8)	O4—O5 <sup>v</sup>	0.858 (7)
As—O8 <sup>v</sup>	1.563 (8)	O5—O5 <sup>v</sup>	1.440 (13)
As—O6	1.6801 (13)	O5—O5 <sup>iv</sup>	1.440 (13)
As—O6 <sup>v</sup>	1.6801 (13)	O5—O7	1.602 (9)
As—O6 <sup>iv</sup>	1.6801 (13)	O6—O8	1.141 (9)
As—O7 <sup>iv</sup>	1.682 (5)	O6—O9 <sup>v</sup>	1.462 (9)
As—O7	1.682 (5)	O6—O7	1.549 (5)
As—O7 <sup>v</sup>	1.682 (5)	O6—O9	1.750 (8)
As—O4	1.693 (2)	O7—O8	1.049 (10)
As—O5 <sup>iv</sup>	1.697 (7)	O7—O9	1.362 (9)
As—O5	1.697 (7)	O8—O9	0.627 (11)
As—O5 <sup>v</sup>	1.697 (7)	O9—O6 <sup>iv</sup>	1.462 (9)
As—O9	1.799 (9)		
O1···O5 <sup>iv</sup>	2.558 (7)	O2···O6 <sup>xvi</sup>	2.7488 (17)
O1···O5	2.612 (8)	O3···O8 <sup>xv</sup>	2.562 (9)
O1···O9 <sup>xv</sup>	2.623 (8)	O3···O6 <sup>xv</sup>	2.6949 (17)
O1···O6 <sup>xvi</sup>	2.6640 (17)	O3···O9 <sup>xv</sup>	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 <sup>xv</sup>	2.919 (5)	O3···O7	2.776 (5)

O2···O9 <sup>xv</sup>	2.515 (9)	O3···O7 <sup>xv</sup>	2.930 (5)
O1 <sup>i</sup> —Sr—O1 <sup>ii</sup>	80.79 (4)	O8 <sup>v</sup> —As—O5 <sup>iv</sup>	140.9 (4)
O1 <sup>i</sup> —Sr—O1 <sup>iii</sup>	80.79 (4)	O6—As—O5 <sup>iv</sup>	128.5 (3)
O1 <sup>ii</sup> —Sr—O1 <sup>iii</sup>	80.79 (4)	O6 <sup>v</sup> —As—O5 <sup>iv</sup>	113.1 (3)
O1 <sup>i</sup> —Sr—O2 <sup>iv</sup>	86.96 (4)	O6 <sup>iv</sup> —As—O5 <sup>iv</sup>	80.9 (3)
O1 <sup>ii</sup> —Sr—O2 <sup>iv</sup>	134.39 (3)	O7 <sup>iv</sup> —As—O5 <sup>iv</sup>	56.6 (3)
O1 <sup>iii</sup> —Sr—O2 <sup>iv</sup>	140.21 (3)	O7—As—O5 <sup>iv</sup>	81.6 (3)
O1 <sup>i</sup> —Sr—O2	140.21 (3)	O7 <sup>v</sup> —As—O5 <sup>iv</sup>	106.7 (3)
O1 <sup>ii</sup> —Sr—O2	86.96 (4)	O8 <sup>iv</sup> —As—O5	140.9 (4)
O1 <sup>iii</sup> —Sr—O2	134.39 (3)	O8—As—O5	91.7 (4)
O2 <sup>iv</sup> —Sr—O2	75.03 (4)	O8 <sup>v</sup> —As—O5	115.8 (4)
O1 <sup>i</sup> —Sr—O2 <sup>v</sup>	134.39 (3)	O6—As—O5	80.9 (3)
O1 <sup>ii</sup> —Sr—O2 <sup>v</sup>	140.21 (3)	O6 <sup>v</sup> —As—O5	128.5 (3)
O1 <sup>iii</sup> —Sr—O2 <sup>v</sup>	86.96 (4)	O6 <sup>iv</sup> —As—O5	113.1 (3)
O2 <sup>iv</sup> —Sr—O2 <sup>v</sup>	75.03 (4)	O7 <sup>iv</sup> —As—O5	106.7 (3)
O2—Sr—O2 <sup>v</sup>	75.03 (4)	O7—As—O5	56.6 (3)
O1 <sup>i</sup> —Sr—O3 <sup>vi</sup>	68.72 (3)	O7 <sup>v</sup> —As—O5	81.6 (3)
O1 <sup>ii</sup> —Sr—O3 <sup>vi</sup>	68.05 (3)	O5 <sup>iv</sup> —As—O5	50.2 (4)
O1 <sup>iii</sup> —Sr—O3 <sup>vi</sup>	138.94 (4)	O8 <sup>iv</sup> —As—O9	80.4 (4)
O2 <sup>iv</sup> —Sr—O3 <sup>vi</sup>	66.55 (3)	O8 <sup>v</sup> —As—O9	108.7 (4)
O2—Sr—O3 <sup>vi</sup>	71.58 (3)	O8—As—O9	19.9 (4)
O2 <sup>v</sup> —Sr—O3 <sup>vi</sup>	134.06 (3)	O6 <sup>v</sup> —As—O9	127.1 (3)
O1 <sup>i</sup> —Sr—O3 <sup>vii</sup>	68.05 (3)	O6—As—O9	60.3 (3)
O1 <sup>ii</sup> —Sr—O3 <sup>vii</sup>	138.94 (4)	O6 <sup>iv</sup> —As—O9	49.6 (3)
O1 <sup>iii</sup> —Sr—O3 <sup>vii</sup>	68.72 (3)	O7 <sup>iv</sup> —As—O9	104.4 (3)
O2 <sup>iv</sup> —Sr—O3 <sup>vii</sup>	71.58 (3)	O7—As—O9	45.9 (3)
O2—Sr—O3 <sup>vii</sup>	134.06 (3)	O7 <sup>v</sup> —As—O9	134.8 (3)
O2 <sup>v</sup> —Sr—O3 <sup>vii</sup>	66.55 (3)	O4—As—O9	123.4 (3)
O3 <sup>vi</sup> —Sr—O3 <sup>vii</sup>	119.992 (1)	O5 <sup>iv</sup> —As—O9	110.0 (4)
O1 <sup>i</sup> —Sr—O3 <sup>viii</sup>	138.94 (4)	O5—As—O9	102.5 (4)
O1 <sup>ii</sup> —Sr—O3 <sup>viii</sup>	68.72 (3)	O5 <sup>v</sup> —As—O9	152.0 (4)
O1 <sup>iii</sup> —Sr—O3 <sup>viii</sup>	68.05 (3)	O8 <sup>iv</sup> —As—O9 <sup>iv</sup>	19.9 (4)
O2 <sup>iv</sup> —Sr—O3 <sup>viii</sup>	134.06 (3)	O8 <sup>v</sup> —As—O9 <sup>iv</sup>	80.4 (4)
O2—Sr—O3 <sup>viii</sup>	66.55 (3)	O8—As—O9 <sup>iv</sup>	108.7 (4)
O2 <sup>v</sup> —Sr—O3 <sup>viii</sup>	71.58 (3)	O6 <sup>v</sup> —As—O9 <sup>iv</sup>	49.6 (3)
O3 <sup>vi</sup> —Sr—O3 <sup>viii</sup>	119.992 (1)	O6—As—O9 <sup>iv</sup>	127.1 (3)
O3 <sup>vii</sup> —Sr—O3 <sup>viii</sup>	119.992 (1)	O6 <sup>iv</sup> —As—O9 <sup>iv</sup>	60.3 (3)
O8 <sup>iv</sup> —As—O8	99.3 (4)	O7 <sup>iv</sup> —As—O9 <sup>iv</sup>	45.9 (3)
O8 <sup>iv</sup> —As—O8 <sup>v</sup>	99.3 (4)	O7—As—O9 <sup>iv</sup>	134.8 (3)
O8—As—O8 <sup>v</sup>	99.3 (4)	O7 <sup>v</sup> —As—O9 <sup>iv</sup>	104.4 (3)

## supplementary materials

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O8 <sup>iv</sup> —As—O6	130.1 (3)	O4—As—O9 <sup>iv</sup>	123.4 (3)
O8 <sup>v</sup> —As—O6	69.2 (3)	O5 <sup>iv</sup> —As—O9 <sup>iv</sup>	102.5 (4)
O8 <sup>iv</sup> —As—O6 <sup>v</sup>	69.2 (3)	O5—As—O9 <sup>iv</sup>	152.0 (4)
O8—As—O6 <sup>v</sup>	130.1 (3)	O5 <sup>v</sup> —As—O9 <sup>iv</sup>	110.0 (4)
O6—As—O6 <sup>v</sup>	109.83 (4)	O9—As—O9 <sup>iv</sup>	92.6 (4)
O8—As—O6 <sup>iv</sup>	69.2 (3)	O8 <sup>iv</sup> —As—O9 <sup>v</sup>	108.7 (4)
O8 <sup>v</sup> —As—O6 <sup>iv</sup>	130.1 (3)	O8 <sup>v</sup> —As—O9 <sup>v</sup>	19.9 (4)
O6—As—O6 <sup>iv</sup>	109.83 (4)	O8—As—O9 <sup>v</sup>	80.4 (4)
O6 <sup>v</sup> —As—O6 <sup>iv</sup>	109.83 (4)	O6 <sup>v</sup> —As—O9 <sup>v</sup>	60.3 (3)
O8—As—O7 <sup>iv</sup>	124.0 (4)	O6—As—O9 <sup>v</sup>	49.6 (3)
O8 <sup>v</sup> —As—O7 <sup>iv</sup>	117.1 (3)	O6 <sup>iv</sup> —As—O9 <sup>v</sup>	127.1 (3)
O6—As—O7 <sup>iv</sup>	164.45 (18)	O7 <sup>iv</sup> —As—O9 <sup>v</sup>	134.8 (3)
O6 <sup>v</sup> —As—O7 <sup>iv</sup>	76.41 (17)	O7—As—O9 <sup>v</sup>	104.4 (3)
O6 <sup>iv</sup> —As—O7 <sup>iv</sup>	54.87 (18)	O7 <sup>v</sup> —As—O9 <sup>v</sup>	45.9 (3)
O8 <sup>iv</sup> —As—O7	117.1 (3)	O4—As—O9 <sup>v</sup>	123.4 (3)
O8 <sup>v</sup> —As—O7	124.0 (4)	O5 <sup>iv</sup> —As—O9 <sup>v</sup>	152.0 (4)
O6—As—O7	54.87 (18)	O5—As—O9 <sup>v</sup>	110.0 (4)
O6 <sup>v</sup> —As—O7	164.45 (18)	O5 <sup>v</sup> —As—O9 <sup>v</sup>	102.5 (4)
O6 <sup>iv</sup> —As—O7	76.41 (17)	O9—As—O9 <sup>v</sup>	92.6 (4)
O7 <sup>iv</sup> —As—O7	117.62 (9)	O9 <sup>iv</sup> —As—O9 <sup>v</sup>	92.6 (4)
O8 <sup>iv</sup> —As—O7 <sup>v</sup>	124.0 (4)	O3 <sup>ix</sup> —Na—O3 <sup>x</sup>	89.64 (5)
O8—As—O7 <sup>v</sup>	117.1 (3)	O3 <sup>ix</sup> —Na—O3 <sup>xi</sup>	89.65 (5)
O6—As—O7 <sup>v</sup>	76.41 (17)	O3 <sup>x</sup> —Na—O3 <sup>xi</sup>	89.64 (5)
O6 <sup>v</sup> —As—O7 <sup>v</sup>	54.87 (18)	O3 <sup>ix</sup> —Na—O2 <sup>xii</sup>	75.47 (4)
O6 <sup>iv</sup> —As—O7 <sup>v</sup>	164.45 (18)	O3 <sup>x</sup> —Na—O2 <sup>xii</sup>	155.21 (3)
O7 <sup>iv</sup> —As—O7 <sup>v</sup>	117.62 (9)	O3 <sup>xi</sup> —Na—O2 <sup>xii</sup>	109.62 (4)
O7—As—O7 <sup>v</sup>	117.62 (9)	O3 <sup>ix</sup> —Na—O2 <sup>xiii</sup>	109.62 (4)
O8 <sup>iv</sup> —As—O4	118.4 (3)	O3 <sup>x</sup> —Na—O2 <sup>xiii</sup>	75.47 (4)
O8—As—O4	118.4 (3)	O3 <sup>xi</sup> —Na—O2 <sup>xiii</sup>	155.21 (3)
O8 <sup>v</sup> —As—O4	118.4 (3)	O2 <sup>xii</sup> —Na—O2 <sup>xiii</sup>	90.76 (5)
O6—As—O4	109.11 (5)	O3 <sup>ix</sup> —Na—O2 <sup>xiv</sup>	155.21 (3)
O6 <sup>v</sup> —As—O4	109.11 (5)	O3 <sup>x</sup> —Na—O2 <sup>xiv</sup>	109.62 (4)
O6 <sup>iv</sup> —As—O4	109.11 (5)	O3 <sup>xi</sup> —Na—O2 <sup>xiv</sup>	75.47 (4)
O7 <sup>iv</sup> —As—O4	81.04 (17)	O2 <sup>xii</sup> —Na—O2 <sup>xiv</sup>	90.76 (5)
O7—As—O4	81.04 (17)	O2 <sup>xiii</sup> —Na—O2 <sup>xiv</sup>	90.76 (5)
O7 <sup>v</sup> —As—O4	81.04 (17)	Na <sup>xvi</sup> —O2—Sr	103.37 (4)
O8 <sup>iv</sup> —As—O5 <sup>iv</sup>	91.7 (4)	Na <sup>xvii</sup> —O3—Sr <sup>xviii</sup>	102.52 (4)
O8—As—O5 <sup>iv</sup>	115.8 (4)		

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)  $z, x, y$ ; (vi)  $-y+1/2, -z, x-1/2$ ; (vii)  $-z, x-1/2, -y+1/2$ ; (viii)  $x-1/2, -y+1/2, -z$ ; (ix)  $-y+1, z+1/2, -x+3/2$ ; (x)  $z+1/2, -x+3/2, -y+1$ ; (xi)  $-x+3/2, -y+1, z+1/2$ ; (xii)  $y+1/2, -z+1/2, -x+1$ ; (xiii)  $-z+1/2, -x+1, y+1/2$ ; (xiv)  $-x+1, y+1/2, -z+1/2$ ; (xv)  $-z+1, x-1/2, -y+1/2$ ; (xvi)  $-x+1, y-1/2, -z+1/2$ ; (xvii)  $-x+3/2, -y+1, z-1/2$ ; (xviii)  $x+1/2, -y+1/2, -z$ .

Fig. 1

