

**Discussion.** Les coordonnées atomiques et les facteurs d'agitation thermique équivalents sont donnés dans le Tableau 1.\* Le Tableau 2 comporte les valeurs des principales distances interatomiques et celles des angles de liaison autour des atomes de molybdène.

La structure de K<sub>2</sub>Th(MoO<sub>4</sub>)<sub>3</sub> s'apparente à celle de la scheelite CaWO<sub>4</sub>. Les atomes de molybdène ont un environnement tétraédrique et se répartissent sur deux sites: Mo(1) est situé sur un axe binaire, Mo(2) est en position générale. La distance moyenne Mo—O (1,779 Å) est comparable à la distance moyenne W—O (1,788 Å) dans CaWO<sub>4</sub> (Kay, Fraser & Almodovar, 1964). Les tétraèdres MoO<sub>4</sub>, isolés les uns des autres, partagent chacun de leurs sommets avec deux autres atomes (K et K ou K et Th ou Th et Th). Chacun des atomes de potassium et de thorium s'entoure ainsi de huit atomes d'oxygène qui forment des dodécaèdres irréguliers liés entre eux par mise en commun de quatre de leurs arêtes (Fig. 1). Comme dans la scheelite, les cations sont regroupés dans des plans (010) distants de  $b/4$ ; toutefois il s'agit ici de plans moyens avec des écarts pour les cations Th<sup>4+</sup>, K<sup>+</sup>, Mo(1)<sup>6+</sup> et Mo(2)<sup>6+</sup>, respectivement égaux à  $y = 0,015, 0,032, -0,252$  et  $0,171$  Å (Fig. 1).

Une projection de la structure selon **b**, sur laquelle ne figurent que les atomes tels que  $0,02 < y < 0,23$  (Fig. 2), fait apparaître les relations géométriques

\* Les listes des facteurs de structure et des facteurs d'agitation thermique anisotrope ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 53434: 12 pp.). On peut en obtenir des copies en s'adressant à: The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

entre les mailles de K<sub>2</sub>Th(MoO<sub>4</sub>)<sub>3</sub> et de CaWO<sub>4</sub> tétragonal:  $\mathbf{a} = \mathbf{a}_t - 3\mathbf{b}_t$ ,  $\mathbf{b} = \mathbf{c}_t$ ,  $\mathbf{c} = -\mathbf{a}_t$ . Par référence à la maille de la scheelite, le triplement du volume de la maille du molybdate double est la conséquence de l'ordonnement des cations K<sup>+</sup> et Th<sup>4+</sup> selon la séquence Th—K—K dans la direction [101] = [010]<sub>t</sub> (Fig. 2). Dans les directions [001] = [100]<sub>t</sub> et [010] = [001]<sub>t</sub>, les périodes ne sont pas modifiées: chacun des plans cationiques (100) contient des ions de même nature. Pour K<sub>2</sub>Th(MoO<sub>4</sub>)<sub>3</sub> la distorsion monoclinique de la structure scheelite apparaît donc comme uniquement la conséquence de la substitution des cations Ca<sup>2+</sup> ( $r = 1,12$  Å) par des ions de charges et de tailles très différentes: K<sup>+</sup> ( $r = 1,51$  Å) et Th<sup>4+</sup> ( $r = 1,05$  Å) (Shannon, 1976).

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## Structure of a Novel Aluminoarsenate with an Occluded (CH<sub>3</sub>)<sub>4</sub>N<sup>+</sup> Cation

BY LI LI\* AND LIXIN WU

*Institute of Theoretical Chemistry, Jilin University, Changchun, People's Republic of China*

AND JIESHENG CHEN AND RUREN XU

*Department of Chemistry, Jilin University, Changchun, People's Republic of China*

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**Abstract.** Trialuminium triarsenate-tetramethylammonium hydroxide (1/1), Al<sub>3</sub>As<sub>3</sub>O<sub>12</sub>·C<sub>4</sub>H<sub>12</sub>N<sup>+</sup>·OH<sup>-</sup>,  $M_r = 588.93$ , monoclinic,  $P2_1/n$ ,  $a = 9.168$  (3),  $b = 19.382$  (6),  $c = 9.779$  (4) Å,  $\beta =$

$115.31$  (3)°,  $V = 1570.9$  (9) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 2.49$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 87.41$  cm<sup>-1</sup>,  $F(000) = 1144$ ,  $T = 298$  K, final  $R = 0.0476$ ,  $wR = 0.0454$  for 2141 reflections with  $I > 4.0\sigma(I)$ . The framework of Al<sub>3</sub>As<sub>3</sub>O<sub>12</sub> contains three types of As atoms and three types of Al atoms. All

\* To whom all correspondence should be addressed.

the As atoms are tetrahedrally coordinated by four O atoms. Of the three types of Al atoms, two types are located in distorted trigonal bipyramids and the third type lies at a tetrahedral centre. Each OH<sup>-</sup> group, which is necessary for balancing the positive charge of the (CH<sub>3</sub>)<sub>4</sub>N<sup>+</sup> cation, bridges two Al atoms. The framework consisting of alternating Al and As atoms has two types of eight-ring channels, one runs along [100] and the other runs along [001]. The (CH<sub>3</sub>)<sub>4</sub>N<sup>+</sup> cations appear in pairs occluded in the channels.

**Introduction.** As molecular sieves, a series of new aluminophosphates occluding quaternary ammonium ions or amines has been extensively investigated (Flanigen, Lok, Patton & Wilson, 1986; Tapp, Milestone & Bibby, 1988; Davis, Saldarriaga, Montes, Garces & Crowder, 1988). Structural characterization showed that they possess frameworks as open as those of zeolites (Parise, 1984; Parise & Day, 1985; Smith, 1988). Several amine-occluding gallophosphates have also been characterized structurally (Parise, 1985, 1986; Yang, Feng & Xu, 1987). Recently, we have investigated the amine-occluding aluminarsenates and galloarsenates (Yang, Li, Chen & Xu, 1989; Chen, Li, Yang & Xu, 1989). However, information about the structures of aluminarsenates or galloarsenates occluding quaternary ammonium ions has never been reported. This article will present the structure of a novel aluminarsenate occluding the tetramethylammonium cation.

**Experimental.** The title compound was obtained by mixing aluminium isopropoxide, pyroarsenic acid, tetramethylammonium hydroxide (TMAOH) and water in the molar ratio of 1:2TMAOH: 1:0Al<sub>2</sub>O<sub>3</sub>: 1:2As<sub>2</sub>O<sub>5</sub>: 40H<sub>2</sub>O, followed by hydrothermal reaction at 475 K for 5 d. A colourless crystal with dimensions 0.10 × 0.15 × 0.25 mm was selected from the product and mounted on a Nicolet R3 four-circle diffractometer. Least-squares fit of 25 strong reflections (15 ≤ θ ≤ 23°) yielded the unit cell and orientation matrix. Intensities were measured by the ω-scan technique with a variable rate of 5.0 to 29.3° min<sup>-1</sup> in the range 3 < 2θ < 72°. A total of 7492 reflections (including 246 standards) were measured, of which 2141 with I<sub>obs</sub> > 4.0σ(I<sub>obs</sub>) were considered as observed and used for structure refinements. Lp and empirical absorption corrections were applied (T<sub>min</sub> = 0.7678, T<sub>max</sub> = 0.9240), as well as a K. B. calculation to obtain absolute intensities. Systematic extinctions led to space group P2<sub>1</sub>/n uniquely.

The positions of the Al and As atoms were obtained by direct-methods calculations, and several cycles of subsequent electron-density syntheses yielded the location of all remaining non-H atoms. The structure refinement on *F* was performed by

Table 1. Atomic coordinates ( $\times 10^4$ ) and temperature factors ( $\text{\AA}^2 \times 10^3$ )

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i>
As(1)	2962 (1)	5733 (1)	3659 (2)	8 (1)*
As(2)	2412 (1)	8042 (1)	4281 (2)	8 (1)*
As(3)	2463 (1)	8074 (1)	-660 (2)	7 (1)*
Al(1)	1369 (3)	9124 (1)	1468 (4)	7 (2)*
Al(2)	3592 (3)	7101 (1)	2299 (4)	8 (2)
Al(3)	49 (3)	6806 (1)	2834 (4)	8 (2)*
O(1)	3721 (6)	6182 (3)	2678 (9)	12 (1)
O(2)	3162 (6)	7370 (3)	431 (9)	14 (1)
O(3)	3843 (6)	7652 (3)	3913 (9)	15 (1)
O(4)	-1169 (6)	6580 (3)	3856 (9)	11 (1)
O(5)	1216 (6)	6028 (3)	3537 (9)	12 (1)
O(6)	844 (7)	7543 (3)	4043 (10)	21 (2)
O(7)	9296 (6)	9274 (3)	490 (9)	16 (1)
O(8)	5784 (6)	7134 (3)	2829 (9)	13 (1)
O(9)	2354 (6)	9918 (3)	1981 (9)	13 (1)
O(10)	2139 (7)	8677 (3)	428 (10)	20 (1)
O(11)	1736 (7)	8748 (3)	3172 (10)	20 (1)
O(12)	8304 (7)	6692 (3)	1037 (10)	19 (1)
O(13)	1303 (6)	7071 (3)	1759 (9)	14 (1)
N(1)	7878 (10)	4394 (4)	1774 (13)	31 (2)
C(1)	6172 (15)	4150 (6)	819 (18)	51 (4)
C(2)	8878 (22)	4437 (9)	884 (25)	107 (7)
C(3)	8621 (21)	3865 (9)	2947 (24)	102 (6)
C(4)	7783 (18)	5066 (8)	2452 (22)	77 (5)

\* Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *U*<sub>ij</sub> tensor.

block-cascade least-squares programs. The coordinates and anisotropic thermal parameters of the Al and As atoms, and the coordinates and isotropic thermal parameters of all remaining non-H atoms were refined, which converged to the final *R* = 0.0476 and *wR* = 0.0454, *w* = 1/σ<sup>2</sup>(*F*), ( $\Delta/\sigma$ ) = 0.10, ( $\Delta\rho$ )<sub>max</sub> = 1.2, ( $\Delta\rho$ )<sub>min</sub> = 0.6 e Å<sup>-3</sup>. All calculations were carried out on an Eclipse S/250 computer using *SHELXTL* programs (Sheldrick, 1978). Scattering factors were those in the *SHELXTL* programs.

**Discussion.** The coordinates of the non-H atoms and equivalent isotropic thermal parameters are given in Table 1,\* and interatomic distances and angles in Table 2.

In the asymmetric unit of the Al<sub>3</sub>As<sub>3</sub>O<sub>12</sub> structure (Fig. 1), there exist three types of As atoms and three types of Al atoms. As with the P atoms in AlPO<sub>4</sub>-*n* or GaPO<sub>4</sub>-*n* (Smith, 1988; Yang, Feng & Xu, 1987), each As atom in Al<sub>3</sub>As<sub>3</sub>O<sub>12</sub> is strictly tetrahedrally coordinated by four O atoms, each of which bridges one Al atom and one As atom. The As—O distances are in the range 1.638–1.691 Å, and O—As—O angles vary from 104.9 to 114.6°. Of the three types of Al atoms, Al(1) lies at the tetrahedral centre, and Al(2) and Al(3) are in distorted trigonal bipyramids.

\* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53044 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Bond lengths (Å) and angles (°)

As(1)—O(1)	1.653 (8)	As(1)—O(5)	1.656 (6)
As(1)—O(7b)	1.683 (7)	As(1)—O(9a)	1.678 (6)
As(2)—O(3)	1.681 (8)	As(2)—O(6)	1.664 (6)
As(2)—O(11)	1.691 (7)	As(2)—O(12b)	1.638 (8)
As(3)—O(2)	1.682 (6)	As(3)—O(10)	1.690 (8)
As(3)—O(4a)	1.660 (7)	As(3)—O(8a)	1.665 (6)
Al(1)—O(9)	1.747 (5)	Al(1)—O(10)	1.702 (10)
Al(1)—O(11)	1.715 (10)	Al(1)—O(7a)	1.749 (6)
Al(2)—O(1)	1.813 (6)	Al(2)—O(2)	1.775 (9)
Al(2)—O(3)	1.836 (9)	Al(2)—O(8)	1.850 (6)
Al(2)—O(13)	1.934 (6)	Al(3)—O(4)	1.841 (9)
Al(3)—O(5)	1.806 (5)	Al(3)—O(6)	1.798 (7)
Al(3)—O(13)	1.930 (10)	Al(3)—O(12a)	1.815 (7)
O(4)—As(3a)	1.660 (7)	O(7)—As(1b)	1.683 (7)
O(7)—Al(1a)	1.748 (6)	O(8)—As(3b)	1.664 (6)
O(9)—As(1a)	1.677 (6)	O(12)—As(2a)	1.638 (8)
O(12)—As(3a)	1.814 (7)	N(1)—C(1)	1.514 (14)
N(1)—C(2)	1.512 (30)	N(1)—C(3)	1.472 (21)
N(1)—C(4)	1.480 (20)		
O(1)—As(1)—O(5)	114.2 (3)	O(1)—As(1)—O(7b)	109.1 (3)
O(5)—As(1)—O(7b)	108.7 (4)	O(1)—As(1)—O(9a)	109.1 (4)
O(5)—As(1)—O(9a)	107.0 (3)	O(7b)—As(1)—O(9a)	108.7 (3)
O(3)—As(2)—O(6)	114.6 (3)	O(3)—As(2)—O(11)	109.4 (4)
O(6)—As(2)—O(11)	108.8 (3)	O(3)—As(2)—O(12b)	106.3 (3)
O(6)—As(2)—O(12b)	110.1 (4)	O(11)—As(2)—O(12b)	107.4 (3)
O(2)—As(3)—O(10)	106.5 (4)	O(2)—As(3)—O(4a)	112.3 (3)
O(10)—As(3)—O(4a)	104.9 (3)	O(2)—As(3)—O(8a)	108.8 (3)
O(10)—As(3)—O(8a)	112.5 (3)	O(4a)—As(3)—O(8a)	111.7 (4)
O(9)—Al(1)—O(10)	108.9 (4)	O(9)—Al(1)—O(11)	103.5 (4)
O(10)—Al(1)—O(11)	113.9 (4)	O(9)—Al(1)—O(7a)	108.5 (3)
O(10)—Al(1)—O(7a)	112.9 (4)	O(11)—Al(1)—O(7a)	108.6 (4)
O(1)—Al(2)—O(2)	117.7 (4)	O(1)—Al(2)—O(3)	115.0 (4)
O(2)—Al(2)—O(3)	127.2 (3)	O(1)—Al(2)—O(8)	90.5 (3)
O(2)—Al(2)—O(8)	90.9 (4)	O(3)—Al(2)—O(8)	91.0 (3)
O(1)—Al(2)—O(13)	89.7 (3)	O(2)—Al(2)—O(13)	89.4 (3)
O(3)—Al(2)—O(13)	88.6 (3)	O(8)—Al(2)—O(13)	179.5 (4)
O(4)—Al(3)—O(5)	89.6 (3)	O(4)—Al(3)—O(6)	90.1 (4)
O(5)—Al(3)—O(6)	113.9 (3)	O(4)—Al(3)—O(13)	178.3 (3)
O(5)—Al(3)—O(13)	92.0 (3)	O(6)—Al(3)—O(13)	88.8 (4)
O(4)—Al(3)—O(12a)	90.5 (4)	O(5)—Al(3)—O(12a)	113.6 (3)
O(6)—Al(3)—O(12a)	132.5 (3)	O(13)—Al(3)—O(12a)	89.3 (4)
As(1)—O(1)—Al(2)	129.0 (5)	As(3)—O(2)—Al(2)	138.4 (5)
As(2)—O(3)—Al(2)	128.5 (3)	Al(3)—O(4)—As(3a)	140.0 (3)
As(1)—O(5)—Al(3)	135.5 (5)	As(2)—O(6)—Al(3)	129.5 (6)
As(1b)—O(7)—Al(1a)	134.9 (6)	Al(2)—O(8)—As(3b)	136.2 (6)
Al(1)—O(9)—As(1a)	137.5 (3)	As(3)—O(10)—Al(1)	163.2 (4)
As(2)—O(11)—Al(1)	146.4 (5)	As(2a)—O(12)—Al(3a)	144.6 (5)
As(2)—O(13)—As(3)	133.6 (4)	C(1)—N(1)—C(2)	112.5 (12)
C(1)—N(1)—C(3)	105.9 (10)	C(2)—N(1)—C(3)	107.1 (13)
C(1)—N(1)—C(4)	107.9 (10)	C(2)—N(1)—C(4)	112.1 (12)
C(3)—N(1)—C(4)	111.1 (13)		

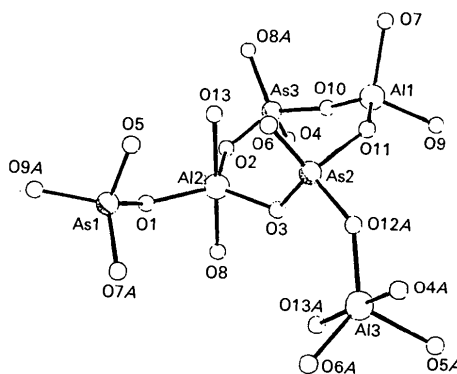
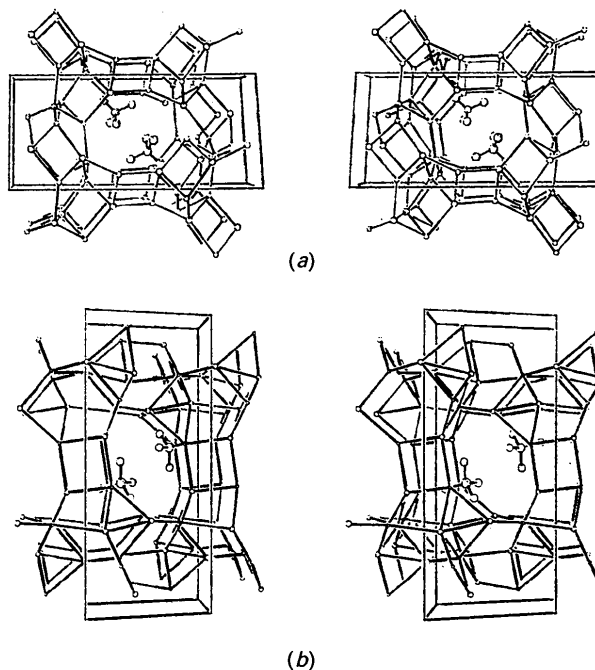
Twelve of the thirteen types of framework O atoms are bonded to one As atom and one Al atom, whereas the thirteenth, representing the position of the OH<sup>-</sup> group, bridges two Al atoms [Al(2) and Al(3)]. The Al(1) tetrahedron is nearly regular: Al(1)—O = 1.702–1.749 Å, O—Al(1)—O = 103.5–113.9°.

There are two sets of Al—O bond lengths in the AlO<sub>5</sub> units (trigonal bipyramids); one is the Al—O (pyramid apex) distance with a range of 1.841–1.934 Å and the other is the Al—O (non-pyramid apex) distance having a range of 1.775–1.836 Å (see Table 2).

Topologically, the three-dimensional framework constructed by the Al, As and O atoms has two

kinds of open channels, as shown in Fig. 2 (O atoms are omitted for clarity). One of the open channels is formed by 8-*T* (*T* = As or Al) rings packing along [100] and the other is formed by 8-*T* rings along [001]. The 8-*T* ring channels are disposed around inversion centres.

The OH<sup>-</sup> groups are necessary for balancing the positive charges of the (CH<sub>3</sub>)<sub>4</sub>N<sup>+</sup> cations. The cations as templates have the proper tetrahedral structure. They are in pairs located in the open 8-*T* ring channels, related by inversion centres.

Fig. 1. Connections in an asymmetric unit of  $\text{Al}_3\text{As}_3\text{O}_{12}$ .Fig. 2. Stereoview of the  $\text{Al}_3\text{As}_3\text{O}_{12}$  framework composed of Al and As nodes along (a) [100] and (b) [001].

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## Er<sub>2</sub>BaNiO<sub>5</sub>: Structure Refinement Using Neutron Powder Diffraction Data

BY J. A. ALONSO, J. AMADOR AND I. RASINES\*

*Instituto de Ciencia de Materiales, CSIC, Serrano 113, 28006 Madrid, Spain*

AND J. L. SOUBEYROUX

*Institut Laue–Langevin, 156 X, 38042 Grenoble CEDEX, France*

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**Abstract.** The crystal structure of erbium barium nickelate, Er<sub>2</sub>BaNiO<sub>5</sub>, has been refined from neutron powder diffraction data, collected at room temperature. Results agree with those obtained from single-crystal X-ray diffraction. Sixfold oxygen coordination around the Ni atoms is confirmed and more precise oxygen positions are given. The NiO<sub>6</sub> octahedra show an unusual twofold distortion: the Ni—O distances to the two axial O atoms are considerably shorter, by 0.3 Å, than those to the four equatorial oxygens; these oxygens are distorted from the right angles of a regular octahedron to 79.1 (1)°. Interesting physical properties are suggested by the existence of infinite isolated chains of NiO<sub>6</sub> flattened octahedra sharing vertices in the direction of the *a* axis, with extremely short, 3.75 Å, Ni—O(axial)—Ni distances. Orthorhombic, *Immm*, *a* = 3.7541 (1), *b* = 5.7442 (1), *c* = 11.3019 (2) Å, *V* = 243.71 (2) Å<sup>3</sup>, *Z* = 2, *λ* = 1.594 Å, *R<sub>wp</sub>* = 7.52%.

**Introduction.** The Nd<sub>2</sub>BaNiO<sub>5</sub> structure type (orthorhombic, *Immm*) was first described by Schiffler & Müller-Buschbaum (1986*a*). Subsequent studies by these authors (Schiffler & Müller-Buschbaum, 1986*a,b*, 1987; Müller-Buschbaum & Lang, 1988; Müller-Buschbaum & Rüter, 1989), established this structure for the compounds formed with rare earth from Sm to Tm. Independently, Amador (1989) pre-

pared and characterized polycrystalline samples of nine R<sub>2</sub>BaNiO<sub>5</sub> oxides, with R = Y, Nd, Sm, Eu, Gd, Dy, Ho, Er or Tm; a better refinement of the Gd<sub>2</sub>BaNiO<sub>5</sub> crystal structure was performed (Amador *et al.*, 1989) and the structure of the yttrium compound was established by single-crystal X-ray diffraction (Amador *et al.*, 1990).

In these compounds, Ni atoms are placed at the centers of flattened oxygen octahedra showing two extremely short Ni—O distances (*i.e.* 1.89 Å for the Gd compound). These polyhedra, rather peculiar in nickel crystallochemistry, particularly contrast with the fivefold oxygen environment of Cu in the iso-stoichiometric compounds R<sub>2</sub>BaCuO<sub>5</sub> (R = Y or rare-earth elements) (Campá *et al.*, 1988), the so-called 'green phases'. The distortions present in the NiO<sub>6</sub> octahedra of the Gd compound (Amador *et al.*, 1989) have recently been shown (Burdett & Mitchell, 1990) to be understandable in terms of a model which combines the results of molecular orbital theory, tight-binding band-structure calculations, and empirical atom–atom potential arguments. In order to check the oxygen stoichiometry and the coordination, especially around Ni atoms, and to confirm both the symmetry and the space group, a neutron powder diffraction study of the erbium compound has been undertaken. The crystal structure of this compound is known (Schiffler & Müller-Buschbaum, 1987), but was determined with a high *R* factor, 0.103.

\* Author to whom correspondence should be addressed.