

Refinement

Refinement on F
 $R = 0.033$
 $wR = 0.037$
 $S = 1.096$
 2226 reflections
 168 parameters
 $(\Delta/\sigma)_{\max} = 0.0006$

$\Delta\rho_{\max} = 0.68 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$
 Extinction correction: Larson (1967)
 Extinction coefficient: 7 (3)
 Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. Selected geometric parameters (\AA , $^\circ$)

V1—O4	2.007 (2)	P1—O1	1.522 (2)
V1—O4 ⁱ	2.007 (2)	P1—O2	1.579 (2)
V1—O6	2.010 (2)	P1—O3	1.538 (2)
V1—O6 ⁱ	2.010 (2)	P1—O4	1.505 (2)
V1—O9	2.022 (2)	P2—O5	1.519 (2)
V1—O9 ⁱ	2.022 (2)	P2—O6	1.528 (2)
V2—O1	1.963 (2)	P2—O7	1.532 (2)
V2—O3 ⁱⁱ	2.022 (2)	P2—O8	1.593 (2)
V2—O5	1.949 (2)	P3—O9	1.534 (2)
V2—O7 ⁱⁱⁱ	2.077 (2)	P3—O10	1.526 (2)
V2—O10 ^{iv}	2.018 (2)	P3—O11	1.494 (2)
V2—O11	1.983 (2)	P3—O12	1.590 (2)
V2—O1—P1	131.8 (1)	V2 ⁱⁱⁱ —O7—P2	124.0 (1)
V2 ⁱⁱ —O3—P1	135.6 (1)	V1—O9—P3	132.1 (1)
V1—O4—P1	162.5 (1)	V2 ^{iv} —O10—P3	139.0 (1)
V2—O5—P2	146.0 (1)	V2—O11—P3	153.8 (1)
V1—O6—P2	130.6 (1)		

Symmetry codes: (i) $-x, 1 - y, 1 - z$; (ii) $1 - x, 1 - y, -z$; (iii) $-x, 2 - y, -z$; (iv) $-x, 1 - y, -z$.

Table 2. Hydrogen-bonding geometry (\AA)

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$
O2—H2 \cdots O9 ⁱ	0.84	1.91	2.742 (3)
O8—H8 \cdots O10 ⁱⁱ	0.82	1.81	2.574 (2)
O12—H12 \cdots O3	0.93	1.80	2.720 (3)
N2—H21 \cdots O8	0.87	2.37	3.025 (4)
N2—H22 \cdots O3 ⁱⁱⁱ	0.82	2.16	2.858 (3)
N2—H23 \cdots O12 ⁱⁱ	0.82	2.14	2.938 (4)
N2—H24 \cdots O6 ⁱ	0.95	2.17	3.060 (4)

Symmetry codes: (i) $1 + x, y, z$; (ii) $x, 1 + y, z$; (iii) $1 - x, 1 - y, 1 - z$.

H-atom parameters were constrained by riding on their O or N partner atoms. Atoms H2, H8, H12, H21, H22 and H23 were located from difference maps, and H24 was placed geometrically [$d(N-H) = 0.95 \text{ \AA}$]. H atoms were refined isotropically. A Tukey–Prince weighting scheme fitted by a three-term Chebychev polynomial with coefficients 0.279, 0.218 and 0.115 was used (Carruthers & Watkin, 1979).

Data collection: *P4 Software* (Siemens, 1995). Cell refinement: *P4 Software*. Data reduction: *P4 Software*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *CRYSTALS* (Watkin, Prout, Carruthers & Betteridge, 1996). Molecular graphics: *CAMERON* (Watkin, Prout & Pearce, 1996) and *ORTEP3* (Farrugia, 1997). Software used to prepare material for publication: *CRYSTALS*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1104). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1998). **C54**, 1197–1200

Ammonium Zinc Vanadium Phosphate, $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$

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Abstract

The title compound, triammonium dizinc vanadium bis(phosphate) bis(hydrogen phosphate), $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$, is the first ammonium zinc vanadium phosphate. It is built up from a three-dimensional network of vertex-sharing VO_6 octahedra and ZnO_4 , PO_4 and HPO_4 tetrahedra fused together via V—O—P and Zn—O—P bonds [$d_{\text{av}}(\text{V—O}) = 2.001(2)$, $d_{\text{av}}(\text{Zn—O}) = 1.949(2)$ and $d_{\text{av}}(\text{P—O}) = 1.538(2) \text{ \AA}$; $\theta_{\text{av}}(\text{V—O—P}) = 142.5$ and $\theta_{\text{av}}(\text{Zn—O—P}) = 131.6^\circ$]. NH_4^+ cations occupy two different types of interstices in the Zn—V—P—O framework.

Comment

Vanadium(III) phosphates have been structurally characterized only recently (Lavrov *et al.*, 1981; Lii *et al.*, 1992; Haushalter *et al.*, 1995). Here, we describe the synthesis and characterization of $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$, the first ammonium zinc vanadium(III) phos-

phate. This phase (Fig. 1) is built up from a three-dimensional framework of VO_6 octahedra and ZnO_4 , PO_4 and HPO_4 tetrahedra sharing vertices as V—O—P and Zn—O—P bonds. Extra-framework NH_4^+ cations complete the structure.

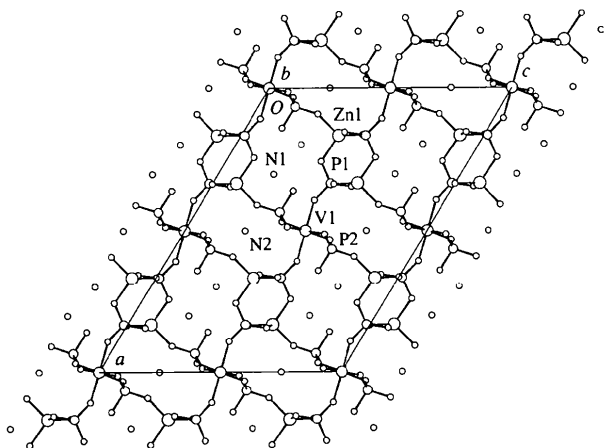


Fig. 1. View of the $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$ structure down $[010]$.

The VO_6 octahedron is close to being regular (the V site symmetry is $\bar{1}$), with $d_{\text{av}}(\text{V—O}) = 2.001(2)$ Å. The bond-valence sum (BVS; Brown, 1996) for this atom is 2.99 [the expected value for vanadium(III) is 3.00]. Other ammonium vanadium(III) phosphates (Haushalter *et al.*, 1995; Bircsak & Harrison, 1998) show a similar, essentially regular, octahedral coordination for the VO_6 grouping, which is quite distinct from the asymmetric coordination favoured by V^{IV} and V^{V} compounds (Jordan & Calvo, 1973; Amorós & Le Bail, 1992). This VO_6 group forms six links to adjacent P atoms, with an average V—O—P bond angle of 142.5° . The ZnO_4 tetrahedron [$d_{\text{av}}(\text{Zn—O}) = 1.949(2)$ Å, $\text{BVS}(\text{Zn}) = 2.07$] is typical for this species (Feng *et al.*, 1997) and forms four Zn—O—P bonds ($\theta_{\text{av}} = 131.6^\circ$). The two phosphate tetrahedra [$d_{\text{av}}(\text{P1—O}) = 1.538(2)$ and $d_{\text{av}}(\text{P2—O}) = 1.539(2)$ Å; $\text{BVS}(\text{P1}) = 4.95$ and $\text{BVS}(\text{P2}) = 4.96$] are also typical. The longer terminal P2—O8 bond suggests that this vertex is protonated (Lightfoot & Masson, 1996). This is supported by the fact that the valence of O8 is 1.06 when considering only its connectivity to P2. P1 makes one P—O—V and three P—O—Zn links; P2 makes two P—O—V links and one P—O—Zn link, and has one terminal P—OH vertex.

The polyhedral connectivity in $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$ may be visualized as the fusing of two types of chains propagating in the $[010]$ direction. The first chain (Fig. 2) consists of a backbone of VO_6 octahedra and P2O_4 tetrahedra. Polyhedral four-rings (two octahedra plus two tetrahedra) arise from this topology, which has also been observed as a building

unit in $\alpha\text{-NH}_4\text{V}(\text{HPO}_4)_2$ (Bircsak & Harrison, 1998) and $\beta\text{-NH}_4\text{V}(\text{HPO}_4)_2$ (Haushalter *et al.*, 1995). A pair of P1O_4 groups are also bound to each V atom in a *trans* configuration.

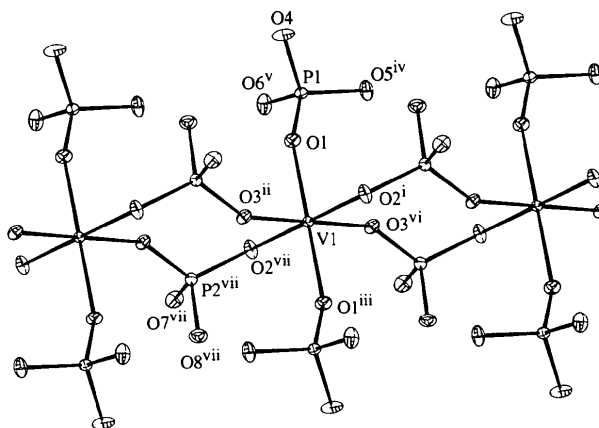


Fig. 2. View of the V—P—O chain in $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$. Displacement ellipsoids are shown at 50% probability. Symmetry codes: (i) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iii) $-x, -y, -z$; (iv) $\frac{1}{2} - x, -\frac{1}{2} - y, -z$; (v) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; (vi) $-\frac{1}{2} + x, -\frac{1}{2} - y, -\frac{1}{2} + z$; (vii) $-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$.

The second chain subunit (Fig. 3) consists of a ladder-like arrangement of edge-sharing four-rings of alternating ZnO_4 and P1O_4 tetrahedra. A hanging P2O_4 group, attached to the Zn centre, completes this chain configuration. This zincophosphate four-ring ladder has a structural precedent in phases such as $\text{CsZn}_3(\text{HPO}_4)_2(\text{PO}_4)$ (Feng *et al.*, 1997) and $\text{H}_3\text{N}(\text{CH}_2)_3\text{NH}_3 \cdot \text{Zn}(\text{HPO}_4)_2$ (Harrison *et al.*, 1998). The ladder-like chains in these phases also contain a hanging phosphate group

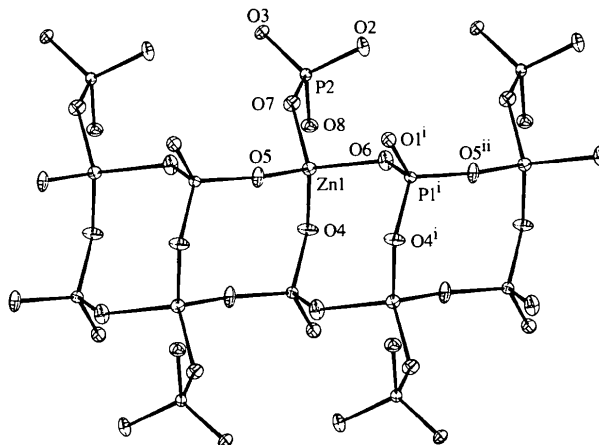


Fig. 3. View of the Zn—P—O chain in $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$. Displacement ellipsoids are shown at 50% probability. Symmetry codes: (i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; (ii) $x, 1 + y, z$.

attached to Zn. The unusual one-dimensional phase $\text{CN}_3\text{H}_6\cdot\text{ZnCl}(\text{HPO}_4)$ (Ng & Harrison, 1998) also contains a four-ring ladder of Zn- and P-centred tetrahedra, with a terminal chloride ion replacing the hanging PO_4 moiety. Similar four-ring ladders are recognized as building units in three-dimensional aluminosilicate zeolite frameworks (Smith, 1988; Feng *et al.*, 1997).

The two distinct ammonium cations occupy voids, visible as small channels propagating in the [010] direction. No details of the hydrogen-bonding situations, if any, of these species could be determined in the present diffraction experiment. If a maximum N...O contact distance of 3.4 Å is assumed, N1 is coordinated by 11 framework O atoms [$d_{\text{av}} = 3.105$ (3) Å] and N2 is coordinated by eight framework O atoms [$d_{\text{av}} = 2.913$ (3) Å].

Experimental

Single crystals of $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$ were synthesized from a mixture of guanidinium carbonate [$(\text{CN}_3\text{H}_6)_2\text{CO}_3$, 0.95 g], ZnO (0.43 g), 85% H_3PO_4 (2.40 g), VCl_3 (0.82 g) and deionized water (7 ml) (starting molar ratio of N:Zn:V:P = 12:1:1:4). The mixture was sealed in a 23 ml Teflon-lined hydrothermal bomb and heated to 453 K for 48 h. After slow cooling, the bomb was opened to reveal a mixture of perfectly faceted yellow-green plates of the title compound (visual yield ~5%), transparent crystals of hopeite [$\text{Zn}_3(\text{PO}_4)_2\cdot 4\text{H}_2\text{O}$] (Whitaker, 1973) and other, unidentified, phases. Syntheses starting from a stoichiometric mixture of precursors, or from a source of ammonium cations, were not successful in preparing $(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$ in measurable yield.

Crystal data

$(\text{NH}_4)_3\text{Zn}_2\text{V}(\text{PO}_4)_2(\text{HPO}_4)_2$	Mo $K\alpha$ radiation
$M_r = 617.72$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 92 reflections
$C2/c$	$\theta = 6-19^\circ$
$a = 20.977$ (3) Å	$\mu = 4.50$ mm ⁻¹
$b = 5.2741$ (4) Å	$T = 298$ K
$c = 15.406$ (2) Å	Faceted plate
$\beta = 121.422$ (7) $^\circ$	$0.4 \times 0.3 \times 0.3$ mm
$V = 1454.5$ (4) Å ³	Yellow-green
$Z = 4$	
$D_x = 2.82$ Mg m ⁻³	
D_m not measured	

Data collection

Siemens P4 diffractometer	$R_{\text{int}} = 0.05$
$2\theta/\omega$ scans	$\theta_{\text{max}} = 32.5^\circ$
Absorption correction:	$h = -1 \rightarrow 31$
ψ scans (North <i>et al.</i> , 1968)	$k = -1 \rightarrow 7$
$T_{\text{min}} = 0.186$, $T_{\text{max}} = 0.263$	$l = -23 \rightarrow 20$
3597 measured reflections	3 standard reflections
2630 independent reflections	every 97 reflections
2630 reflections with $I > 0$	intensity decay: none

Refinement

Refinement on F	$\Delta\rho_{\text{max}} = 0.90$ e Å ⁻³
$R = 0.038$	$\Delta\rho_{\text{min}} = -0.80$ e Å ⁻³
$wR = 0.036$	Extinction correction:
$S = 1.92$	Larson (1967)
2630 reflections	Extinction coefficient:
121 parameters	38.9 (17)
H atoms not located	Scattering factors from <i>International Tables for X-ray Crystallography</i> (Vol. IV)
$w_i = 1/[\sigma^2(F_o)]$	
$(\Delta/\sigma)_{\text{max}} = 0.0007$	

Table 1. Selected geometric parameters (Å, $^\circ$)

Zn1—O4	1.984 (2)	P1—O4	1.548 (2)
Zn1—O5	1.920 (2)	P1—O5 ⁱⁱⁱ	1.539 (2)
Zn1—O6	1.951 (2)	P1—O6 ^{ix}	1.537 (2)
Zn1—O7	1.942 (2)	P2—O2	1.530 (2)
V1—O1	2.000 (2)	P2—O3	1.512 (2)
V1—O2 ⁱ	1.996 (2)	P2—O7	1.521 (2)
V1—O3 ⁱⁱ	2.008 (2)	P2—O8	1.593 (2)
P1—O1	1.529 (2)		
V1—O1—P1	146.4 (1)	Zn1—O5—P1 ⁱⁱⁱ	133.9 (1)
V1 ⁱⁱ —O2—P2	135.6 (1)	Zn1—O6—P1 ^{iv}	127.2 (1)
V1 ⁱ —O3—P2	145.5 (1)	Zn1—O7—P2	143.1 (1)
Zn1—O4—P1	122.2 (1)		

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

Data collection: *P4 Software* (Siemens, 1995). Cell refinement: *P4 Software*. Data reduction: *P4 Software*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *CRYSTALS* (Watkin, Prout, Carruthers & Betteridge, 1996). Molecular graphics: *CAMERON* (Watkin, Prout & Pearce, 1996). Software used to prepare material for publication: *CRYSTALS*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1102). Services for accessing these data are described at the back of the journal.

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AsO_4 (Fig. 1). Chaque chaîne $[\text{TiO}(\text{AsO}_4)_2]_n$ est liée à quatre voisines situées à des distances Ti—Ti de 7,72 et 7,94 Å, au moyen de liaisons Na—O (Fig. 2).

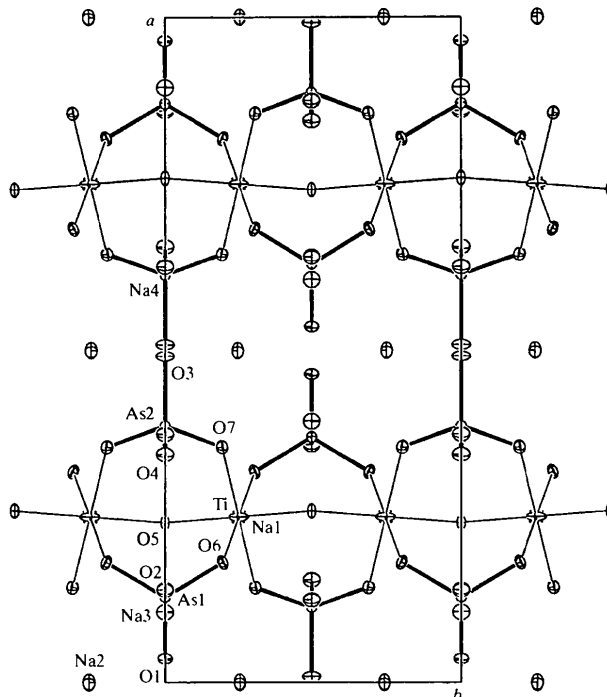


Fig. 1. Projection de la structure de $\text{Na}_4\text{TiAs}_2\text{O}_9$ sur le plan (001). Les ellipsoïdes de vibration des atomes ont une probabilité de 50%.

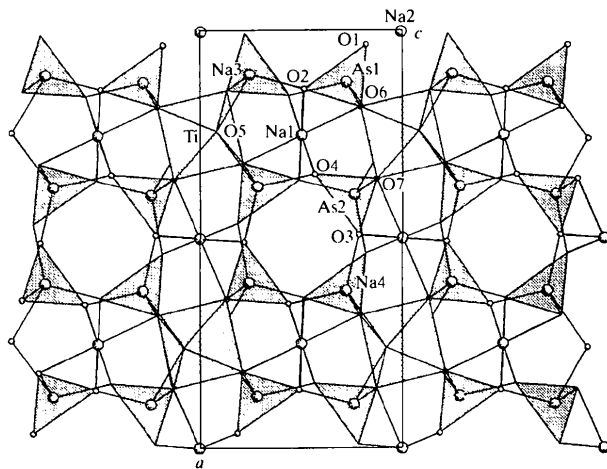


Fig. 2. Projection de la structure de $\text{Na}_4\text{TiAs}_2\text{O}_9$ sur le plan (010).

Les colonnes $[\text{TiO}(\text{AsO}_4)_2]_n$ ménagent entre elles trois types de tunnels partiellement occupés par les ions sodium. Les cations Na1 et Na2 sont situés respectivement dans les sites 4f ($\bar{1}$) et 4g (2) sur les axes des tunnels limités par deux chaînes voisines.

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$\text{Na}_4\text{TiAs}_2\text{O}_9$

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(Reçu le 27 février 1997, accepté le 22 décembre 1997)

Abstract

The three-dimensional framework of tetrasodium titanium nonaoxodarsenate, $\text{Na}_4\text{TiAs}_2\text{O}_9$, consists of infinite $[\text{TiO}(\text{AsO}_4)_2]_n$ chains linked together by Na^+ cations. The structure is compared with those of $\text{Na}_3\text{SbO}(\text{PO}_4)_2$ ($P2_12_12_1$) and $\text{Na}_4\text{TiP}_2\text{O}_9$ ($P2/c$, *Ibam* and *Bmcm*).

Commentaire

Les études effectuées dans les systèmes ternaires $\text{A}_2\text{O}-\text{TiO}_2-\text{As}_2\text{O}_5$ ont permis d'isoler la série de formulation $\text{ATi}_2(\text{AsO}_4)_3$ ($A = \text{Li, Na, K et Ag}$) (Yaakoubi *et al.*, 1991) de type Nasicon caractérisé par une conductivité ionique élevée (Hagman & Kierkegaard, 1968) et les composés ATiOAsO_4 ($A = \text{alcalin}$). Ces derniers adoptent trois types de structures: LiTiOAsO_4 (Robertson *et al.*, 1994) a une charpente tridimensionnelle analogue à celle de $\beta\text{-LiVOPO}_4$ (Lii *et al.*, 1991), le titanyl-arséniate de sodium et de potassium $\text{Na}_{0,87}\text{K}_{0,13}\text{TiOAsO}_4$ (Phillips *et al.*, 1992) isotype de CaTiOSiO_4 (Donnay & Ondik, 1973) et de NaVOAsO_4 (Haddad *et al.*, 1992), et enfin les composés KTiOAsO_4 (El Brahimy & Durand, 1986), CsTiOAsO_4 (Protas *et al.*, 1989), RbTiOAsO_4 (Thomas *et al.*, 1992) et $\text{Ag}_{0,98}\text{K}_{0,02}\text{TiOAsO}_4$ (Phillips *et al.*, 1992) isostructuraux de KTiOPO_4 (Tordjman *et al.*, 1974) connu pour ses propriétés optiques de doubleur de fréquence (Zumesteg *et al.*, 1976). Le présent travail est consacré à la préparation et à l'étude structurale de $\text{Na}_4\text{TiO}(\text{AsO}_4)_2$.

La structure renferme des chaînes d'octaédres TiO_6 , parallèles à $[010]$, partageant des sommets. Deux octaédres successifs sont bridés par deux tétraédres