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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{As}-\text{O}) = 0.002$ Å
 R factor = 0.009
 wR factor = 0.023
Data-to-parameter ratio = 9.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Xenotime-type $\text{Yb}[\text{AsO}_4]$

$\text{Yb}[\text{AsO}_4]$, ytterbium(III) oxoarsenate(V), adopts the xenotime structure type. Single crystals were obtained in an attempt to synthesize a compound with nominal composition $\text{Yb}_3\text{OCl}[\text{AsO}_3]_2$ by fusing a mixture of Yb_2O_3 , YbCl_3 and As_2O_3 in a 4:1:3 molar ratio at 1123 K, owing to air-intrusion during the reaction. The structure is built up by chains of edge-sharing $[\text{YbO}_8]$ trigonal dodecahedra and $[\text{AsO}_4]$ tetrahedra in a primitive rod packing. Yb and As are situated on positions with $\bar{4}m2$ symmetry, whereas O atoms are located on a mirror plane.

Comment

$\text{Yb}[\text{AsO}_4]$ adopts the xenotime structure and is isotypic with all known rare earth(III) oxoarsenates(V) $M[\text{AsO}_4]$ ($M = \text{Sc}$, Sm, Tb–Ho and Lu; Schäfer & Will, 1971; Lohmüller *et al.*, 1973; Schäfer *et al.*, 1979; Schmidt, *et al.*, 2005; Kang & Schleid, 2005) and oxophosphates(V) $M'[\text{PO}_4]$ ($M' = \text{Sc}$, Y and Tb–Lu; Milligan *et al.*, 1983; Ni *et al.*, 1995) that crystallize in this structure type.

The structure contains one single ytterbium site where the Yb^{3+} cations are coordinated by eight O atoms forming two interpenetrating tetrahedra, a compressed and an elongated one [$\text{Yb}-\text{O} = 2.2584$ (18) and 2.3910 (18) Å]. The resulting coordination figure can thus be described as a trigonal dodecahedron (Fig. 1). These $[\text{YbO}_8]$ polyhedra share four edges each. The As^{V} cations are coordinated by four O atoms in the shape of a slightly distorted tetrahedron [$\text{As}-\text{O} = 1.6831$ (17) Å and $\text{O}-\text{As}-\text{O} = 98.49$ (12)° (2×) and 115.23 (7)° (4×)]. The oxoarsenate(V) tetrahedra share *trans* edges with the elongated and all vertices with the compressed subtetrahedra within the $[\text{YbO}_8]$ trigonal dodecahedra (Fig. 2).

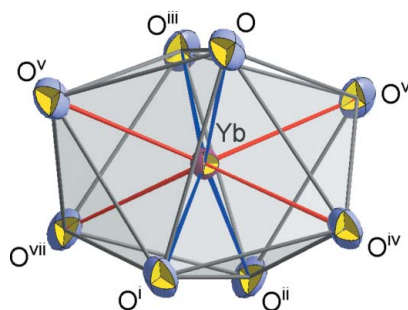


Figure 1

The trigonal-dodecahedral coordination sphere of the Yb^{3+} cation, built by two interpenetrating tetrahedra, an elongated one (red bonds) and a compressed one (blue bonds). Displacement ellipsoids are drawn at the 95% probability level. [Symmetry codes: (i) $y - \frac{3}{4}, x + \frac{3}{4}, -z + \frac{1}{4}$; (ii) $-x, -y + \frac{3}{2}, z$; (iii) $-y + \frac{3}{4}, x + \frac{3}{4}, -z + \frac{1}{4}$; (iv) $y - \frac{1}{4}, -x + \frac{3}{4}, z + \frac{1}{4}$; (v) $-x, -y + 1, -z$; (vi) $-y + \frac{1}{4}, -x + \frac{3}{4}, z + \frac{1}{4}$; (vii) $x, y + \frac{1}{2}, -z$.]

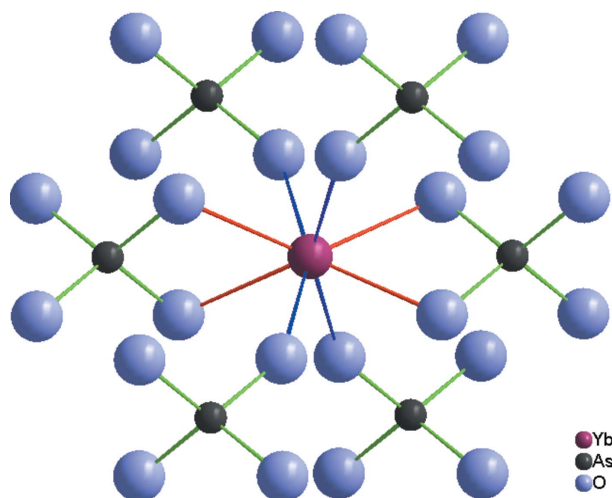


Figure 2
Each $[\text{YbO}_8]$ polyhedron is connected to six $[\text{AsO}_4]$ tetrahedra, two edge- and four vertex-attached ones.

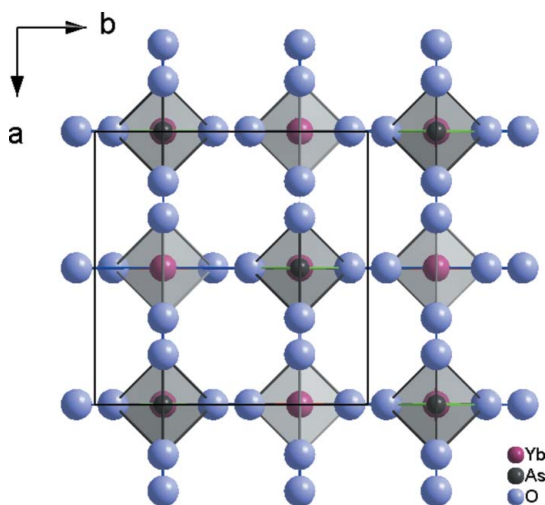


Figure 3
The crystal structure of $\text{Yb}[\text{AsO}_4]$, viewed along $[001]$. The chains of alternating $[\text{YbO}_8]$ trigonal dodecahedra and $[\text{AsO}_4]$ tetrahedra are arranged in a primitive rod packing. For a better view, only the elongated (red bonds) subtetrahedra within the $[\text{YbO}_8]$ trigonal dodecahedra are drawn.

Through their shared edges, the $[\text{AsO}_4]$ and $[\text{YbO}_8]$ units build up chains along $[001]$. The structure created by the chains of alternating $[\text{YbO}_8]$ polyhedra and $[\text{AsO}_4]$ tetrahedra can be described as a primitive rod packing (Fig. 3). Another way to describe the structure emphasizes a three-dimensional framework arranged by the edge-shared $[\text{YbO}_8]$ polyhedra alone, with the oxoarsenate(V) tetrahedra residing in channels along $[111]$ (Fig. 4).

Experimental

Single crystals of $\text{Yb}[\text{AsO}_4]$ were obtained in attempts to synthesize a compound with nominal composition $\text{Yb}_3\text{OCl}[\text{AsO}_3]_2$ by fusing a mixture of Yb_2O_3 , YbCl_3 and As_2O_3 in a 4:1:3 molar ratio at 1123 K for 7 d in flame-sealed evacuated silica ampoules. CsCl was used as a

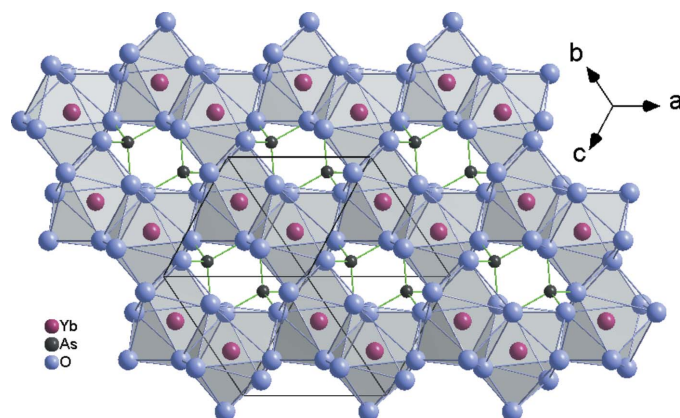


Figure 4
The crystal structure of $\text{Yb}[\text{AsO}_4]$, viewed along $[111]$. The oxoarsenate(V) units reside in channels of the $[\text{YbO}_8]$ -polyhedra framework.

flux to improve the crystal growth. The ampoules were cooled to room temperature over a period of 4 d. Instead of $\text{Yb}_3\text{OCl}[\text{AsO}_3]_2$, in analogy with $\text{Gd}_3\text{OCl}[\text{AsO}_3]_2$ (Kang *et al.*, 2005), the product consisted of minor amounts of YbOCl (Brandt & Diehl, 1974) and the title compound (main product) owing to air-intrusion during the reaction, and therefore further oxidation of the As^{III} component to As^{V} .

Crystal data

$\text{Yb}[\text{AsO}_4]$
 $M_r = 311.96$
Tetragonal, $I4_1/amd$
 $a = 6.9712$ (4) Å
 $c = 6.2431$ (4) Å
 $V = 303.40$ (3) Å³
 $Z = 4$
 $D_x = 6.830$ Mg m⁻³

Mo $K\alpha$ radiation
Cell parameters from 1512 reflections
 $\theta = 4.4\text{--}28.3^\circ$
 $\mu = 41.46$ mm⁻¹
 $T = 293$ (2) K
Block, colourless
 $0.07 \times 0.06 \times 0.04$ mm

Data collection

Nonius KappaCCD diffractometer
 φ and ω scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1999)
 $T_{\text{min}} = 0.082$, $T_{\text{max}} = 0.174$
2463 measured reflections
114 independent reflections

109 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 28.3^\circ$
 $h = -9 \rightarrow 9$
 $k = -9 \rightarrow 9$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.009$
 $wR(F^2) = 0.023$
 $S = 1.06$
114 reflections
12 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 0.1746P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.13$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.56$ e Å⁻³
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0122 (5)

Table 1

Selected geometric parameters (Å, °).

Yb—O	2.2584 (18)	As—O	1.6831 (17)
Yb—O ^{iv}	2.3910 (18)		
O ^{viii} —As—O	115.23 (7)	O ^{ix} —As—O	98.49 (12)

Symmetry codes: (iv) $y - \frac{1}{4}, -x + \frac{3}{4}, z + \frac{1}{4}$; (viii) $y - \frac{1}{4}, x + \frac{1}{4}, -z + \frac{3}{4}$; (ix) $-x, -y + \frac{1}{2}, z$.

For the present refinement, the centrosymmetric setting for space group $I4_1/amd$ with origin choice 2 was selected. The highest peak in the final difference Fourier map is located 0.79 Å from Yb.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXL97*.

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