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Synthetic mansfieldite, $AlAsO_4{\cdot}2H_2O$

William T. A. Harrison

Department of Chemistry, University of Aberdeen, Aberdeen AB24 3UE, Scotland
Correspondence e-mail: w.harrison@abdn.ac.uk

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Hydrothermally prepared mansfieldite, $AlAsO_4{\cdot}2H_2O$ (aluminium arsenate dihydrate), contains a vertex-sharing three-dimensional network of *cis*-$AlO_4(H_2O)_2$ octahedra and AsO_4 tetrahedra [d_{av}(Al—O) = 1.907 (2) Å, d_{av}(As—O) = 1.685 (2) Å and θ_{av}(Al—O—As) = 134.5 (1)°].

Comment

On the basis of cell parameters, symmetry and composition, the present phase is a synthetic analogue of mansfieldite, $AlAsO_4{\cdot}2H_2O$ (Allen *et al.*, 1948; Ronis & D'Yvoire, 1969). Mansfieldite is a member of the $M^{III}XO_4{\cdot}2H_2O$ (M = Al, Fe, Ga, Cr; X = P, As) family of phases exemplified by variscite, $AlPO_4{\cdot}2H_2O$ (Kniep *et al.*, 1977).

The *cis*-$AlO_4(H_2O)_2$ octahedron [d_{av}(Al—O) = 1.907 (2) Å] and AsO_4 tetrahedron [d_{av}(As—O) = 1.685 (2) Å] share vertices, as Al—O—As bonds [atoms O1–O4 with θ_{av} = 134.5 (1)°], resulting in a three-dimensional network of polyhedra. Three of the four water H atoms participate in O—H···O hydrogen bonds in a similar manner to that seen in variscite (Kniep *et al.*, 1977).

Experimental

A starting mixture of KOH (1 *M*, 4 ml), $Al(NO_3)_3$ (0.5 *M*, 8 ml) and H_3AsO_4 (1 *M*, 4 ml) was heated to 443 K in a 23-ml-capacity teflon-lined hydrothermal bomb for 4 d. Upon cooling the bomb to ambient temperature over a period of 2–3 h, a crop of small (to 0.1 mm) blocks and octahedra of the title compound was recovered by vacuum filtration and washing with water and acetone.

Crystal data

$AlAsO_4{\cdot}2H_2O$
M_r = 201.93
Orthorhombic, *Pbca*
a = 8.8218 (5) Å
b = 9.8252 (6) Å
c = 10.1163 (6) Å
V = 876.8 (2) Å^3
Z = 8
D_x = 3.06 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2390 reflections
θ = 3.70–30.66°
μ = 7.89 mm^{-1}
T = 298 K
Faceted block, colourless
0.08 × 0.08 × 0.08 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.470, T_{max} = 0.532
8491 measured reflections
1587 independent reflections
1059 reflections with $I > \sigma(I)$
R_{int} = 0.039
θ_{max} = 32.5°
$h = -12 \rightarrow 9$
$k = -14 \rightarrow 11$
$l = -14 \rightarrow 11$

Refinement

Refinement on F
R = 0.025
wR = 0.026
S = 1.047
1059 reflections
90 parameters
All H-atom parameters refined
Weighting: Chebychev polynomial with 3 parameters (Carruthers & Watkin, 1979): 0.139, 0.174, 0.091
$(\Delta/\sigma)_{max}$ = 0.000112
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Al1—O1	1.903 (2)	Al1—O6	1.977 (3)
Al1—O2^{i}	1.883 (3)	As1—O1	1.684 (2)
Al1—O3^{ii}	1.894 (2)	As1—O2	1.679 (2)
Al1—O4^{iii}	1.866 (3)	As1—O3	1.685 (2)
Al1—O5	1.920 (3)	As1—O4	1.692 (2)
Al1—O1—As1	133.20 (13)	Al1^{v}—O3—As1	135.42 (14)
Al1^{iv}—O2—As1	135.50 (15)	Al1^{iii}—O4—As1	133.99 (14)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H51···O4^{i}	0.82 (8)	1.78 (8)	2.592 (3)	169 (8)
O5—H52···O1^{ii}	0.72 (6)	2.04 (6)	2.729 (3)	160 (6)
O6—H62···O3	0.94 (7)	1.70 (7)	2.578 (4)	155 (7)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SMART*; program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1997); software used to prepare material for publication: *CRYSTALS*.

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