Crystal structure of hexasodium trizinc tetraarsenate trihydrate, Na₆Zn₃(AsO₄)₄ · 3H₂O

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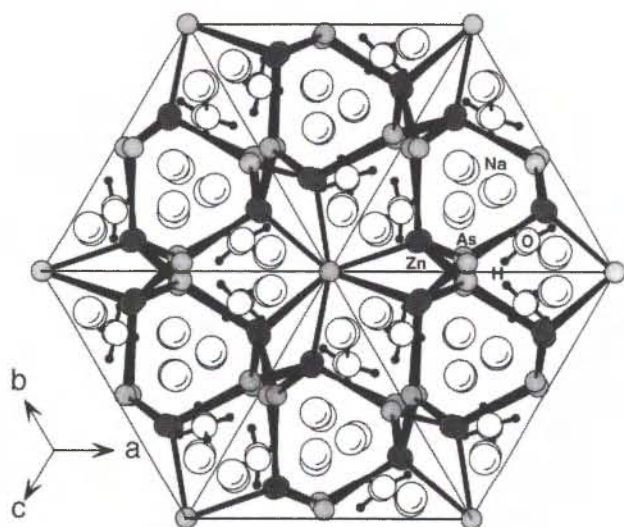
Abstract

As₄H₆Na₆O₁₉Zn₃, cubic, $P2_13$ (No. 198), $a = 12.245(1)$ Å, $V = 1836.0$ Å^3, $Z = 4$, $R_{gt}(F) = 0.018$, $R_w(F^2) = 0.036$, $T = 300$ K.

Source of material

The material was crystallised from NaOH, ZnO, H₃AsO₄ and H₂O under hydrothermal conditions at 533 K with autogeneous pressure for 130 h in a teflon coated steel autoclave under static conditions.

Discussion

The compound was described by Grey et al. [1] together with its relation to garnet. The crystal structure is built up by ZnO₄ and AsO₄ tetrahedra. In the figure, the oxygen atoms are not drawn for clarity. The sodium atoms are octahedrally coordinated by five tetrahedra oxygen atoms and the oxygen atoms of the water molecule (O9). The hydrogen atoms form hydrogen bridging bonds to the two tetrahedra oxygen atoms O2 (H91: 191.8 pm) and O4 (H92: 199.3 pm). The mean metal-oxygen distances are 248 pm for Na1 and Na2, 194 pm for Zn1 and 168 pm – 169 pm for the different As atoms.

Table 1. Data collection and handling.

Crystal:	colorless, cube-shaped, size 0.10 x 0.10 x 0.10 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	132.96 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 140 exposures, $\Delta\varphi = 1.7°$
$2\theta_{max}$:	56.5°
$N(hkl)_{measured}$, $N(hkl)_{unique}$.	20984, 1508
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1338
$N(param)_{refined}$:	105
Programs:	STRUCTURE TIDY [2], SHELXS-86 [3], SHELXL-93 [4], DIAMOND [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(91)	12b	0.035(4)	0.179(2)	0.375(5)	0.06(1)
H(92)	12b	0.068(3)	0.299(4)	0.389(5)	0.06(1)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
As(1)	4a	0.03146(2)	x	x	0.0055(1)	U_{11}	U_{11}	0.0000(1)	U_{12}	U_{12}
As(2)	4a	0.26905(3)	x	x	0.0047(1)	U_{11}	U_{11}	0.0005(1)	U_{12}	U_{12}
As(3)	4a	0.51778(2)	x	x	0.0051(1)	U_{11}	U_{11}	0.0004(1)	U_{12}	U_{12}
As(4)	4a	0.77878(3)	x	x	0.0056(1)	U_{11}	U_{11}	0.0002(1)	U_{12}	U_{12}
Zn(1)	12b	0.12491(3)	0.49148(3)	0.24714(3)	0.0061(2)	0.0073(2)	0.0073(2)	0.0004(1)	0.0014(1)	0.0002(1)
Na(1)	12b	0.9943(1)	0.2431(1)	0.1722(1)	0.0188(7)	0.0110(6)	0.0183(7)	−0.0010(5)	0.0019(6)	−0.0011(5)
Na(2)	12b	0.2457(1)	0.4206(1)	0.5020(1)	0.0196(8)	0.0225(7)	0.0099(6)	−0.0026(5)	−0.0028(5)	−0.0006(5)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	12b	0.0099(2)	0.5440(2)	0.3380(2)	0.012(1)	0.021(1)	0.011(1)	0.006(1)	0.006(1)	0.003(1)
O(2)	12b	0.0550(2)	0.4205(2)	0.1187(2)	0.013(1)	0.009(1)	0.009(1)	0.0013(9)	−0.0039(9)	0.0001(9)
O(3)	12b	0.1940(2)	0.2292(2)	0.5953(2)	0.015(1)	0.017(1)	0.013(1)	0.006(1)	−0.0038(9)	−0.008(1)
O(4)	12b	0.1981(2)	0.3735(2)	0.3263(2)	0.014(1)	0.010(1)	0.009(1)	0.0052(9)	0.0022(9)	−0.0017(9)
O(5)	4a	0.1916(2)	x	x	0.0134(8)	U_{11}	U_{11}	−0.0020(9)	U_{12}	U_{12}
O(6)	4a	0.4397(2)	x	x	0.0149(9)	U_{11}	U_{11}	−0.0026(9)	U_{12}	U_{12}
O(7)	4a	0.7009(2)	x	x	0.0148(8)	U_{11}	U_{11}	−0.0031(9)	U_{12}	U_{12}
O(8)	4a	0.9535(2)	x	x	0.0150(8)	U_{11}	U_{11}	−0.0037(9)	U_{12}	U_{12}
O(9)	12b	0.0046(2)	0.2523(2)	0.3764(2)	0.024(2)	0.022(2)	0.026(1)	−0.001(1)	−0.000(1)	0.002(1)

References

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