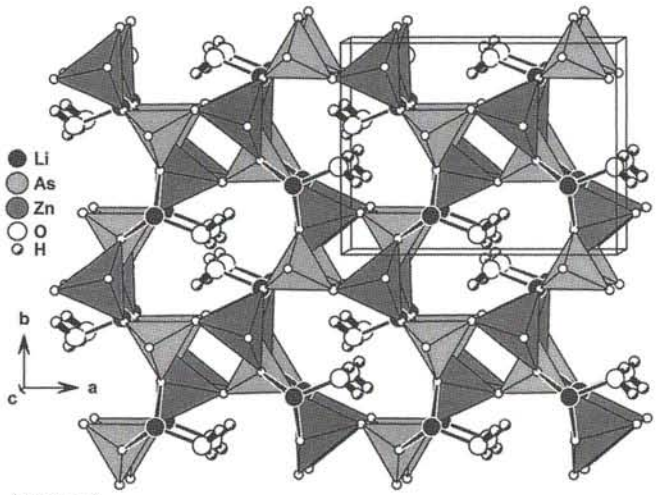
Crystal structure of lithium zinc arsenate hydrate, $LiZnAsO_4 \cdot H_2O$

Th. M. Gesing*

Universität Hannover, Institut für Mineralogie, Welfengarten 1, D-30167 Hannover, Germany

Received January 7, 1999, transferred to 2nd update of database ICSD in 1999, CSD-No. 409396



Abstract

AsH_2LiO_5Zn, orthorhombic, $Pna2_1$ (No. 33), $a = 10.861(1)$ Å, $b = 8.2955(9)$ Å, $c = 5.1568(5)$ Å, $V = 464.6$ Å^3, $Z = 4$, $R_p = 0.047$, $wR_p = 0.064$, $R(I) = 0.012$, $T = 293$ K.

Source of material

The material was prepared from single crystals of $NaZnAsO_4 \cdot 2H_2O$ in a half concentrated lithium chloride solution at room temperature. After 21 days rod like polycrystals of $LiZnAsO_4 \cdot H_2O$ remaind together with a rest of 7% of $NaZnAsO_4 \cdot 2H_2O$.

The lattice constant were refined from Guinier powder data with α-quartz ($a = 491.30$ pm, $c = 540.46$ pm) as internal standard. The refinement was carried out with $NaZnAsO_4 \cdot 2H_2O$ as a second phase with a refined amount of 7%. Starting atomic coordinates were taken from $LiZnAsO_4 \cdot D_2O$ [1]. The hydrogen atoms were restrained to the water molecule oxygen atom (O5) with a distance of 96 pm during the refinement. The displacement parameters were fixed.

Discussion

In the course of our work on sodium zink arsenates [2] we carried out ion exchange experiments which lead in the case of lithium salts to the formation of $LiZnAsO_4 \cdot H_2O$ together with small amounts of the starting arsenate material. For we wanted to know the distribution of the two phases in the sample and the crystal structure of $LiZnAsO_4 \cdot H_2O$ was not investigated until now we refined the structure from X-ray powder data. A refinement of a single crystal was not possible caused by multiple twinning. The existence of this compound together with lattice parameters was described by Harrison et al. [3]. The crystal structure of $LiZnAsO_4 \cdot H_2O$ is built up by ZnO_4 and AsO_4 tetrahedra which form a three dimensional network with 8-ring channels along the [001] direction. Secondary building units are single four- and six-rings. The tetrahedrally coordinated lithium atoms are placed in the 6-rings whereas the oxygen atoms are located in the 8-ring channels. One hydrogen atom of the water molecule forms very weak hydrogen bridging bond to the framework oxygen atom O1 (H1: 222 pm). This is confirmed by IR spectroscopy. The mean metal-oxygen distances are 170 pm, 192 pm and 195 pm for the arsenic, lithium and zinc atoms, respectively.

Table 1. Data collection and handling.

Powder:	colourless, grounded crystals
Wavelength:	Cu K_α radiation (1.5406 Å)
μ:	1.23 cm^{-1}
Diffractometer:	Stoe Stadi P
Scan mode:	transmission Debye-Scherrer mode
$2\theta_{max}$, stepwidth:	89.98°, 0.02
$N(points)_{measured}$:	4000
$N(hkl)_{measured}$:	217
$N(param)_{refined}$:	54
Programs:	RIETAN-97 [4], Diamond [5]

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

Atom	Site	x	y	z	U_{iso}
Li	4a	0.318(4)	0.179(5)	0.78(2)	0.02(2)
As	4a	0.1721(3)	0.0766(4)	1/4[a]	0.017(1)
Zn	4a	0.3761(3)	0.3687(4)	0.260(2)	0.018(1)
O(1)	4a	0.040(2)	0.177(2)	0.177(4)	0.019(7)
O(2)	4a	0.296(2)	0.173(2)	0.133(4)	0.024(9)
O(3)	4a	0.192(2)	0.065(3)	0.582(4)	0.030(8)
O(4)	4a	0.166(2)	0.890(2)	0.125(3)	0.014(7)
O(5)	4a	0.484(2)	0.091(2)	0.76(1)	0.062(6)
H(1)	4a	0.54(2)	0.17(2)	0.82(5)	0.024
H(2)	4a	0.51(3)	0.05(4)	0.59(4)	0.024

a: arbitrarily fixed for definition of the origin.

References

1. Norby, P.; Norlund Christensen, A. N.; Andersen, I. G. K.: Hydrothermal preparation of Zeolite Li-A(BW), LiAlSiO4 · H2O and structure determination from powder diffraction data by direct methods. Acta. Chem. Scan. **40** (1986) 500-506.
2. Gesing, Th. M.: Structure and Properties of the layer compound $NaZnAsO_4 \cdot 2\ H_2O$. Z. Kristallogr. **213** (1998) 386-391.
3. Harrison, W. T. A.; Gier, T. E.; Nicol, J. M.; Stucky, G. D.: TetrahedralFramework Lithium Zinc Phosphate Phases: Location of light-Atom Positions in $LiZnPO_4(H_2O)$ by Powder Neutron Diffraktion and Structure Determination by ab Initio Methods. J. Solid State Chem. **114** (1995) 249 -257.
4. Izumi, F.: "The Rietveld Method", ed. by R. A. Young, Oxford University Press, Oxford 1993.
5. Brandenburg, K: DIAMOND. Visual information system for crystal structures. University of Bonn, Germany 1996.

* Correspondence author
(e-mail: tm.gesing@mineralogie.uni-hannover.de)