

Acta Cryst. (1971). **B27**, 1837

The crystal structure of SnHAsO₄. By ALAN F. BERNDT, *Chemistry Department, University of Missouri—St. Louis, St. Louis, Missouri 63121, U.S.A.*

(Received 9 March 1971)

Compound SnHAsO₄ is isostructural with SnHPO₄. The unit cell is monoclinic with $a=4.777 \pm 0.012$, $b=14.153 \pm 0.049$, $c=6.024 \pm 0.025$ Å, $\beta=100^\circ 15' \pm 30'$. Space group is $P2_1/c$, and the density calculated for $Z=4$ is 4.29 g.cm⁻³.

The reaction between solutions of SnCl₂·2H₂O and Na₂HAsO₄·7H₂O was studied at various values of pH and for Sn:As ratios between 1:2 and 3:2. Identical X-ray powder patterns were given by the crystalline precipitate in every case. Single crystals of this product were obtained by a diffusion-controlled reaction. A sample of SnCl₂·2H₂O was placed in one leg of an 'H' shaped tube filled with water. Crystals of Na₂HAsO₄·7H₂O were placed in the other leg, and the reaction mixture was maintained under an argon atmosphere. Numerous needle-like crystals were observed after several days.

A crystal approximately 0.01 mm in diameter and 0.2 mm in length was chosen for data collection and was mounted with the long dimension coincident with the axis of rotation. Multiple-film equi-inclination Weissenberg data were collected for layers $hk0$ through $hk3$ with Ni-filtered Cu $K\alpha$ radiation ($\lambda=1.54178$ Å). Comparison of the observed intensity data with that previously reported for SnHPO₄ (Berndt & Lamberg, 1971) clearly indicates the isomorphism between these two compounds. If the isomorphism is complete, then the product of the reaction

between SnCl₂·2H₂O and Na₂HAsO₄·7H₂O is SnHAsO₄. The unit cell of SnHAsO₄ is monoclinic with

$$\begin{aligned} a &= 4.777 \pm 0.012 \text{ \AA} \\ b &= 14.153 \pm 0.049 \\ c &= 6.024 \pm 0.025 \\ \beta &= 100^\circ 15' \pm 30' . \end{aligned}$$

Lattice constants were determined from a powder pattern indexed with the aid of the single-crystal data. Standard deviations in the lattice constants were estimated by a least-squares analysis. The density calculated for $Z=4$ is 4.29 g.cm⁻³, and the space group is $P2_1/c$.

Although SnHPO₄ and SnHAsO₄ are isostructural they do not have identical crystalline habits. Both compounds crystallize as needles; however, the needle axis of SnHPO₄ is [103] (Berndt & Lamberg, 1971), whereas the needle axis of SnHAsO₄ is [001].

References

BERNDT, A. F. & LAMBERG, R. (1971). *Acta Cryst.* **B27**, 1092.

Acta Cryst. (1971). **B27**, 1837

Errata in *International Tables for X-ray Crystallography*. By A. D. MIGHELL, A. SANTORO and J. D. H. DONNAY, *National Bureau of Standards, Washington D.C. 20234, U.S.A.*

(Received 7 June 1971)

A number of misprints in *International Tables for X-ray Crystallography* (1969), Vol. I should be corrected.

The following misprints should be corrected in *International Tables for X-Ray Crystallography*, Vol. I (1969) reprinting:

Table 5.1.2.1

Last item in condition 4(a)

$$\text{For } |\mathbf{a} \cdot \mathbf{b}| \leq \frac{1}{2} \mathbf{a} \cdot \mathbf{a} \text{ read } |\mathbf{a} \cdot \mathbf{b}| \leq \frac{1}{2} \mathbf{a} \cdot \mathbf{a}$$

Conditions (5c), (5d), (5e)

$$\begin{aligned} \text{For } \mathbf{b} \cdot \mathbf{c} = \frac{1}{2} \mathbf{b} \cdot \mathbf{b} & \text{ read } |\mathbf{b} \cdot \mathbf{c}| = \frac{1}{2} \mathbf{b} \cdot \mathbf{b} \\ \mathbf{a} \cdot \mathbf{c} = \frac{1}{2} \mathbf{a} \cdot \mathbf{a} & \text{ read } |\mathbf{a} \cdot \mathbf{c}| = \frac{1}{2} \mathbf{a} \cdot \mathbf{a} \\ \mathbf{a} \cdot \mathbf{b} = \frac{1}{2} \mathbf{a} \cdot \mathbf{a} & \text{ read } |\mathbf{a} \cdot \mathbf{b}| = \frac{1}{2} \mathbf{a} \cdot \mathbf{a} \end{aligned}$$

Table 5.1.2.2

Matrix of cell S, sixth entry

$$\text{For } \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{b} & \mathbf{a} \cdot \mathbf{c} & \mathbf{a} \cdot \mathbf{b} \end{pmatrix} \text{ read } \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \\ -\frac{\mathbf{b} \cdot \mathbf{b}}{2} & \mathbf{a} \cdot \mathbf{c} & \mathbf{a} \cdot \mathbf{b} \end{pmatrix}$$

Matrix of cell S, seventh entry

$$\text{For } \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{c} & \mathbf{a} \cdot \mathbf{a} & \mathbf{a} \cdot \mathbf{b} \end{pmatrix} \text{ read } \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{c} & -\frac{\mathbf{a} \cdot \mathbf{a}}{2} & \mathbf{a} \cdot \mathbf{b} \end{pmatrix}$$

Matrix of cell S', sixth entry

$$\begin{aligned} \text{For } \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{b} & (|\mathbf{a} \cdot \mathbf{c}| + |\mathbf{a} \cdot \mathbf{b}|) & |\mathbf{a} \cdot \mathbf{b}| \end{pmatrix} \\ \text{read } \begin{pmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{b} & (|\mathbf{a} \cdot \mathbf{c}| + |\mathbf{a} \cdot \mathbf{b}|) & |\mathbf{a} \cdot \mathbf{b}| \end{pmatrix} \end{aligned}$$

Relations between scalars, last entry

$$\text{For } 2|\mathbf{a} \cdot \mathbf{c}| + 2|\mathbf{a} \cdot \mathbf{b}| < \mathbf{a} \cdot \mathbf{a} \text{ read } 2|\mathbf{a} \cdot \mathbf{c}| + |\mathbf{a} \cdot \mathbf{b}| < \mathbf{a} \cdot \mathbf{a}$$

Transformation matrix, last entry

$$\text{For } 100/010/111 \text{ read } \bar{1}00/0\bar{1}0/111$$

Table 5.1.3.1

Entry No. 8

$$\text{For } c_1 = [a(\mathbf{a} \cdot \mathbf{a} - |\mathbf{b} \cdot \mathbf{c}|)]^{1/2} \text{ read } c_1 = [2(\mathbf{a} \cdot \mathbf{a} - |\mathbf{b} \cdot \mathbf{c}|)]^{1/2}$$

Entry No. 15

$$\text{For } c_1 = [2(c^2 - a^2)]^{1/2} \text{ read } c_1 = [2(2c^2 - a^2)]^{1/2}$$

Entry No. 18

$$\text{For } \frac{a \cdot a}{2} \quad \frac{a \cdot a}{2} \quad \frac{a \cdot a}{2} \quad \text{read} \quad \frac{a \cdot a}{4} \quad \frac{a \cdot a}{2} \quad \frac{a \cdot a}{2}$$

Entry No. 19

$$\text{For } c_1 = [2b^2 - a^2 + b \cdot c]^{1/2} \quad \text{read} \quad c_1 = [2b^2 - a^2 + 2b \cdot c]^{1/2}$$

Entry No. 30

$$\text{For } a_1 = a, c_1 = b \quad \text{read} \quad a_1 = b, c_1 = a$$

Entry No. 43 third fraction

$$\text{For } -\frac{|a \cdot b|}{2} \quad \text{read} \quad -|a \cdot b|$$

The last correction was pointed out to us by Mr Massoud Behruzi, Diplom-Mineralog, Aachen, Germany (BRD).

References

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

International Union of Crystallography

Journal of Applied Crystallography* Acta Crystallographica*

Journal of Applied Crystallography

The Executive Committee of the International Union of Crystallography announces that it is necessary to increase the regular yearly subscription rates for the *Journal of Applied Crystallography* from 1 January 1972. The subscription rates have remained constant since the journal was launched in 1968 although the number of papers submitted has increased substantially and the size of the volume for 1971 is likely to be nearly twice that for 1969. It is also necessary to cover the continued increases in the basic costs of production.

The new yearly subscription rates for 1972 (Volume 5) are:

Complete volumes, regular price per volume
D.kr. 300 (\$40.50 or £16.90)

Complete volumes, reduced price for individuals
D.kr. 150 (\$20.25 or £8.45)

Single parts
D.kr. 75 (\$10.00 or £4.20)

At the present rates of exchange, orders are also accepted in U.S. dollars and pounds sterling at the prices shown in parentheses. Orders should be addressed to Munksgaard International Publishers Ltd., Nørre Søgade 35, 1370 Copenhagen K, Denmark or to any bookseller. Orders for complete volume from subscribers in the North American area may alternatively be placed through Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pa. 15238, U.S.A. at the U.S. dollar prices shown above. The reduced rate subscriptions for individuals are ordinarily only available to members of recognized scientific societies, who must give a written undertaking accompanying their subscription application that the journal is for their personal use and will not be made available to libraries, institutions, etc.

Each annual volume of the journal contains six parts, except Volume 1 (1968) which contained only five parts. The prices for back numbers published before 1 January 1972 (Volumes 1-4) will remain unaltered. At the present rates of exchange these prices are:

* *Note added in proof:* - Owing to recent variations in exchange rates the dollar prices given here no longer apply.

Complete volumes, regular price per volume
D.kr. 240 (\$32.40 or £13.50)

Complete volumes, reduced price for individuals
D.kr. 120 (\$16.20 or £6.75)

Single parts
D.kr. 60 (\$8.10 or £3.40)

Acta Crystallographica

The prices for *Acta Crystallographica* remain unaltered. The yearly subscription rates are:

Complete volumes, regular price per volume
Combined subscription,
Sections A & B D.kr. 1000 (\$135.00 or £56.25)
Section A only D.kr. 250 (\$33.75 or £14.05)
Section B only D.kr. 850 (\$114.75 or £47.80)

Complete volumes, reduced price for individuals
Combined subscription,
Sections A & B D.kr. 400 (\$54.00 or £22.50)
Section A only D.kr. 100 (\$13.50 or £5.60)
Section B only D.kr. 340 (\$45.90 or £19.10)

Single parts
Section A D.kr. 60 (\$8.10 or £3.40)
Section B D.kr. 100 (\$13.50 or £5.60)

Each annual volume of Section A (crystal physics, diffraction, theoretical and general crystallography) contains six parts and each annual volume of Section B (structural crystallography and crystal chemistry) contains twelve parts.

The prices for back numbers published before 1 January 1972 also remain unchanged. For a full list of these prices see *Acta Cryst.* (1969) A25, 718, *Acta Cryst.* (1969) B25, 2172 or *J. Appl. Cryst.* (1969) 2, 191.

Eighth General Assembly and International Congress of Crystallography

A full report of the Eighth General Assembly of the International Union of Crystallography, held at the State University of New York at Stony Brook, U.S.A. from 13 to 21 August 1969, and of the Eighth International Congress of Crystallography, has been published in the September 1971 issue of *Acta Crystallographica*, Vol. A27, page 497.