Acta Cryst. (1971). B**27**, 1837

The crystal structure of $SnHAsO_4$.

By ALAN F. BERNDT, *Chemistry Department, University of Missouri–St. Louis, St. Louis, Missouri* 63121, *U.S.A.*

(*Received* 9 *March* 1971)

Compound $SnHAsO_4$ is isostructural with $SnHPO_4$. The unit cell is monoclinic with $a=4{\cdot}777\pm0{\cdot}012$, $b=14{\cdot}153\pm0{\cdot}049$, $c=6{\cdot}024\pm0{\cdot}025$ Å, $\beta=100°15'\pm30'$. Space group is $P2_1/c$, and the density calculated for $Z=4$ is 4·29 g.cm^{-3}.

The reaction between solutions of $SnCl_2.2H_2O$ and $Na_2HAsO_4.7H_2O$ was studied at various values of *p*H 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 $SnCl_2.2H_2O$ was placed in one leg of an '*H*' shaped tube filled with water. Crystals of $Na_2HAsO_4.7H_2O$ 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 *hk*0 through *hk*3 with Ni-filtered Cu $K\alpha$ radiation ($\lambda=1{\cdot}54178$ Å). Comparison of the observed intensity data with that previously reported for $SnHPO_4$ (Berndt & Lamberg, 1971) clearly indicates the isomorphism between these two compounds. If the isomorphism is complete, then the product of the reaction between $SnCl_2.2H_2O$ and $Na_2HAsO_4.7H_2O$ is $SnHAsO_4$.

The unit cell of $SnHAsO_4$ is monoclinic with

$$\begin{aligned} a &= 4{\cdot}777\pm0{\cdot}012 \text{ Å} \\ b &= 14{\cdot}153\pm0{\cdot}049 \\ c &= 6{\cdot}024\pm0{\cdot}025 \\ \beta &= 100°15'\pm30'. \end{aligned}$$

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 $SnHPO_4$ and $SnHAsO_4$ are isostructural they do not have identical crystalline habits. Both compounds crystallize as needles; however, the needle axis of $SnHPO_4$ is [$\bar{1}$03] (Berndt & Lamberg, 1971), whereas the needle axis of $SnHAsO_4$ is [001].

References

BERNDT, A. F. & LAMBERG, R. (1971). *Acta Cryst.* B**27**, 1092.

Acta Cryst. (1971). B**27**, 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*)

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

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

For		read	
	$\mathbf{b}\cdot\mathbf{c}=\frac{1}{2}\mathbf{b}\cdot\mathbf{b}$		$\lvert\mathbf{b}\cdot\mathbf{c}\rvert=\frac{1}{2}\mathbf{b}\cdot\mathbf{b}$
	$\mathbf{a}\cdot\mathbf{c}=\frac{1}{2}\mathbf{a}\cdot\mathbf{a}$		$\lvert\mathbf{a}\cdot\mathbf{c}\rvert=\frac{1}{2}\mathbf{a}\cdot\mathbf{a}$
	$\mathbf{a}\cdot\mathbf{b}=\frac{1}{2}\mathbf{a}\cdot\mathbf{a}$		$\lvert\mathbf{a}\cdot\mathbf{b}\rvert=\frac{1}{2}\mathbf{a}\cdot\mathbf{a}$

Table 5.1.2.2

Matrix of cell **S**, sixth entry

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

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

For $\begin{pmatrix}\mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \frac{\mathbf{b}\cdot\mathbf{b}}{2} & (|\mathbf{a}\cdot\mathbf{c}|+|\mathbf{a}\cdot\mathbf{b}) & |\mathbf{a}\cdot\mathbf{b}|\end{pmatrix}$

read $\begin{pmatrix}\mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \frac{\mathbf{b}\cdot\mathbf{b}}{2} & (|\mathbf{a}\cdot\mathbf{c}|+|\mathbf{a}\cdot\mathbf{b}|) & |\mathbf{a}\cdot\mathbf{b}|\end{pmatrix}$

Relations between scalars, last entry

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

Transformation matrix, last entry

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

Table 5.1.3.1

Entry No. 8

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

Entry No. 15

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

Entry No. 18