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Lattice parameters of Zn_3As_2.

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Rotation and precession data taken using a single crystal of Zn_3As_2 indicate a body-centered tetragonal unit cell. Lattice parameters obtained from spectrometer measurements on a single crystal with faces cut perpendicular to (001) and (100) give

$$c = 23{\cdot}65,\ a = 11{\cdot}78\ \text{Å}.$$

This cell is $4\times2\times2$ times larger than the originally reported cubic cell (Natta & Passerini, 1928), and $2\times\sqrt{2}\times\sqrt{2}$ times larger than the previously reported tetragonal cell (Stackelberg & Paulus, 1935). With $c/a = 2{\cdot}007$ this material is highly pseudo-cubic and is one of the few good intermetallic semiconductors which is not actually cubic. The space group is probably $I4_1/acd$. There was a great deal of difficulty with preferred orientation in the powder patterns. Fig. 1 shows the first few lines in the powder pattern obtained using Ni-filtered Cu radiation and linear recording. The strong lines in this pattern agree with those reported by Natta & Passerini.

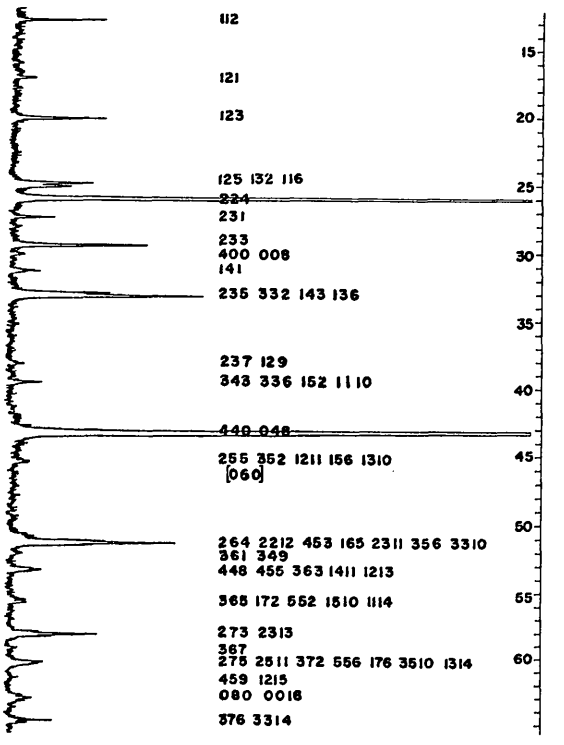

Fig. 1. Powder pattern of Zn_3As_2; filtered Cu radiation.

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The crystal structure of mercury(II)oxide.

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A determination of the crystal structure of mercury(II)-oxide, recently reported by Roth (1956) and carried out on the basis of X-ray and neutron diffraction powder data, is inconsistent with observations previously published by the present author (Aurivillius, 1954) and also with supplementary data obtained later on. Weak, interspacing layer lines in the X-ray rotation photographs of single crystals of mercury(II)oxide taken around [100] show the actual a axis to be twice that first reported by Zachariasen (1927) and supported by Roth. The Weissenberg photograph of the first interspacing layer line ($1kl$, Cu $K\alpha$ radiation) thus shows 18 independent reflexions (cf. Table 1) which should be absent according to the structure proposed by Roth. The doubling of the a axis has been confirmed by amply exposed X-ray pow-

Table 1. *Observed intensities* $1kl$ *from a Weissenberg photograph of* HgO *and calculated structure-factor values*

	$k=$	0	1	2	3	4	5	6
$l=1$	I_o	w^+	w	w	—	—	—	—
	$F^2/10$	43	9	27	0·2	12	0·3	6
$l=2$	I_o	w^+	—	w^+	—	w	vw	w
	$F^2/10$	38	0·3	30	0·8	17	1	12
$l=3$	I_o	w	w	w	w	w	w	—
	$F^2/10$	18	12	16	10	13	9	—
$l=4$	I_o	w	w^+	w	w^+	—	—	—
	$F^2/10$	6	41	9	37	—	—	—

Table 2. *Part of the powder photograph of* HgO

Cu $K\alpha_1$ radiation

Indices referred to the unit cell found at the present investigation

	$10^4 \times \sin^2\theta$		Present investigation		Roth	
hkl	Obs.	Calc.	I_o	$(pF^2)_c \times 10^{-3}$	I_o	I_c
200	544	543	*vw*	2·2	—	—
101	615	614	*vw*	1·8	—	—
011	673	673	*vst*	280	424	425
210	737	737	*vst*	240	353	346
020	778	779	*vst*	170	236	221
111	807	809	*vvw*	0·7	—	—
201	1021	1021	*vst*	290	275	272
211	1215	1216	*w*	9·5	—	—
220	1320	1322	*vw*	3·7	—	—
121	1393	1393	*vw*	2·2	—	—
301	1704	1700	*vvw*	1·0	—	—
221	1798	1800	*vst*	480	206	209
311	—	1895	—	0·03	—	—
002	1914	1914	*st*	110	39	40
102	2047	2050	*vvw*	1·5	—	—
400	2170	2171	*st*	110	39	39
031	2231	2231	*st*	200	56	56
112	—	2244	—	0·03	—	—
230	2295	2295	*st*	180	54	54
410 }	2363	2366	*w*	{ 15	—	—
131 }		2366		{ 0·2		

der photographs taken in a Guinier focusing camera (Table 2).

The following structure, derived from powder and single-crystal data obtained by X-ray and neutron diffraction methods, is in reasonable agreement with the experimental results.

Cell content: 4 HgO.
Cell dimensions: $a = 6{\cdot}612_1$, $b = 5{\cdot}520_1$, $c = 3{\cdot}521_3$ Å.
Space group: *Pnma* (No. 62).
4 Hg in (*c*): $x, \frac{1}{4}, z; \bar{x}, \frac{3}{4}, \bar{z}; \frac{1}{2}-x, \frac{3}{4}, \frac{1}{2}+z; \frac{1}{2}+x, \frac{1}{4}, \frac{1}{2}-z$ with $x = 0{\cdot}115$, $z = 0{\cdot}245$.
4 O in (*c*): with $x = 0{\cdot}36_5$, $z = 0{\cdot}58_5$.

This structure is built up of infinite planar zigzag chains running parallel to the *a* axis and lying in the *ac* plane. Within the chains the distance Hg–O is $2{\cdot}03 \pm 0{\cdot}10$ Å and the angles O–Hg–O and Hg–O–Hg are $179 \pm 3°$ and $109 \pm 1°$ respectively. This chain arrangement is essentially different from that found by Roth, the principal divergence being the bonding of the oxygen atoms to the mercury atoms, the angle O–Hg–O given by Roth being 110°.

A full report will appear in *Acta Chemica Scandinavica*.

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The structural crystallography of indium bismuthide.*

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From X-ray crystallographic analysis the unit cell of the intermetallic compound InBi is found to be tetragonal with dimensions $a = b = 5{\cdot}000$, and $c = 4{\cdot}773$ Å. Absent X-ray spectra and the presence of a center of symmetry are consistent with the space group $P4/nmm$. Density measurements show that there are two molecules of InBi in the unit cell so that the atoms are at special positions, the coordinates of which are (0, 0, 0), $(\frac{1}{2}, \frac{1}{2}, 0)$ and $(0, \frac{1}{2}, z)$, $(\frac{1}{2}, 0, \bar{z})$. By employing the observed intensities of (0*kl*) reflections in summations of the Patterson and Fourier types, the In atoms are located at the origin and the end-centered position, while the unknown coordinate, *z*, is found to be 0·393. The reliability index of this analysis, expressed in the usual manner, is 0·17.

Fig. 1 shows four unit cells of InBi and also the tetrahedral array of four Bi atoms around each In atom with the dimensions and angles listed. Each Bi atom has four In atoms as nearest neighbours, forming a square to one side of it. The structure consists of layers of like atoms normal to the *c* axis with adjacent In layers separated by two Bi layers. Each In layer is bonded to the Bi layer on either side of it and the closest approach of the Bi

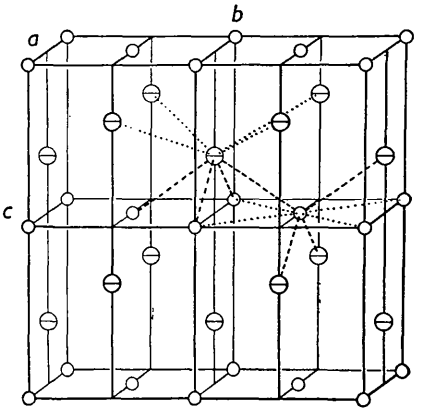

Fig. 1. Atomic arrangement in four unit cells of InBi.

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