

*Acta Cryst.* (1956). **9**, 685

**Lattice parameters of  $Zn_3As_2$ .** By H. COLE, F. W. CHAMBERS and H. M. DUNN, *IBM Research Laboratory, Poughkeepsie, New York, U.S.A.*

(Received 8 May 1956 and in revised form 4 June 1956)

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

$$c = 23.65, a = 11.78 \text{ \AA}.$$

This cell is  $4 \times 2 \times 2$  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  $c/a = 2.007$  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  $I4_1acd$ . 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.

#### References

- NATTA, G. & PASSERINI, L. (1928). *Gazz. chim. ital.*, **58**, 541.  
 STACKELBERG, M. V. & PAULUS, R. (1935). *Z. phys. Chem. B*, **28**, 427.

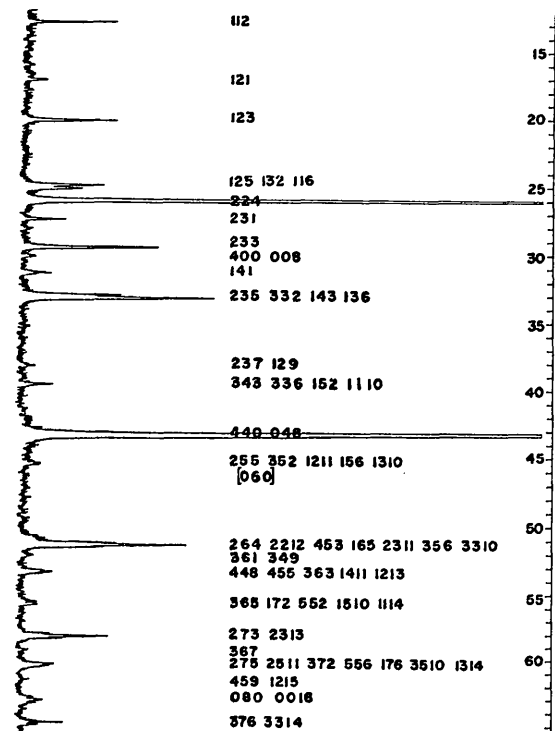


Fig. 1. Powder pattern of  $Zn_3As_2$ ; filtered Cu radiation.

*Acta Cryst.* (1956). **9**, 685

**The crystal structure of mercury(II)oxide.** By KARIN AURIVILLIUS, *Institute of Inorganic and Physical Chemistry, University of Stockholm, Sweden, and Joint Establishment of Nuclear Energy Research, Kjeller, Norway*

(Received 23 April 1956 and in revised form 23 May 1956)

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 Zachariassen (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
$l=2$	$I_o$	$w^+$	—	$w^+$	—	$w$	$w$	$w$
	$F^2/10$	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	—	—	—