Acta Cryst. (1962). **15**, 94

The crystal structure of Sc_3In.

By V. B. Compton and B. T. Matthias, *Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A.*

(*Received* 11 *August* 1961 *and in revised form* 28 *September* 1961)

Ferromagnetism in the scandium–indium system is being investigated by Matthias, Clogston, Williams, Corenzwit & Sherwood (1961). The crystal structure of the compound Sc_3In is reported here.

An ingot was prepared by reacting Sc and In in the proportions 3·15 to 1 in an arc furnace under an argon atmosphere and then annealing the sample at 800 °C. for one week. X-ray diffraction photographs were taken of the resulting product using a Norelco camera of 114·6 mm. diameter and Cu K-radiation ($\lambda = 1{\cdot}5418$ Å). The pattern resembled that of scandium with somewhat smaller lattice constants. However, the presence of some extra lines suggested the possibility of a superlattice. To investigate this, filings of the melt were annealed at 390 °C. for two weeks. The powder diffraction pattern of this material could be indexed on a hexagonal lattice with

$$a = 6{\cdot}421 \pm 0{\cdot}005,\ c = 5{\cdot}183 \pm 0{\cdot}005\ \text{Å}\ .$$

The observed and calculated interplanar spacings are listed in Table 1. There are two extremely weak extra lines which are probably due to another phase in the Sc–In system.

Table 1. *Comparison of observed and calculated interplanar spacings and intensities*

$hk{\cdot}l$	d_o	d_c	I_o*	I_c
10·0	5·539 Å	5·561 Å	*m*	100
10·1	3·770	3·791	*s*	244
11·0	3·187	3·211	*m*	108
20·0	2·763	2·780	*vs*	245
00·2	2·585	2·592	*vs*	265
20·1	2·449	2·450	*vvs*	1000
11·2	2·010	2·017	*w*	61
21·1	1·945	1·948	*w–m*	83
20·2	1·888	1·896	*m–s*	150
22·0	1·603	1·605	*m–s*	166
31·1	1·475	1·478	*vvw*	34
20·3	1·463	1·467	*s*	183
22·2	1·361	1·365	*s*	191
40·1	1·341	1·343	*m–s*	136
40·2	1·222	1·225	*vw*	33
40·3	1·082	1·083	*w–m*	72
42·1	1·029	1·030	*m–s*	127
22·4	1·008	1·008	*m*	85
42·2	0·9710	0·9739	*m*	42
20·5		0·9713		61
60·0	0·9271	0·9268	*vw* (diffuse)	42
42·3	0·8973	0·8978	*m–s*	127
60·2	0·8726	0·8727	*m*	91
40·5	0·8317	0·8311	*m*	84
42·4	0·8169	0·8162	*w–m*	64

* Visually estimated

(*vs* = very strong; *s* = strong; *m* = medium; *w* = weak).

To conserve space, calculated intensities below 30 are omitted.

Relative intensities were calculated based on a Mg_3Cd type structure (DO_{19}) which is a superlattice derived from hexagonal close-packing (Wells, 1950). The presence of a superlattice was suggested by the fact that the axial length a is approximately twice that of Sc.

The Mg_3Cd structure was determined by Dehlinger (1930). The space group is D^4_{6h}–$P6_3/mmc$ with two formula weights per unit cell. The atom positions are:

6Sc in (h); $x, 2x, \frac{1}{4};\ 2\bar{x}, \bar{x}, \frac{1}{4};\ x, \bar{x}, \frac{1}{4};\ \bar{x}, 2\bar{x}, \frac{3}{4};\ 2x, x, \frac{3}{4};$
$\bar{x}, x, \frac{3}{4};\ x = \frac{5}{6}$.
2In in (c); $\frac{1}{3}, \frac{2}{3}, \frac{1}{4};\ \frac{2}{3}, \frac{1}{3}, \frac{3}{4}$.

The intensities were computed for $x = 0{\cdot}823$, 0·833 and 0·843. The best agreement between calculated and observed intensities, visually estimated, is obtained for $x = 0{\cdot}833$. The results are given in Table 1. The low intensity of the low angle lines is probably due to absorption. Satisfactory agreement between the observed and calculated intensities confirmed the Mg_3Cd type structure for Sc_3In.

The structure consists of 4 A3 type (h.c.p.) unit cells in which $\frac{1}{4}$ of the Sc atoms are replaced by In. In this structure the nearest neighbors to an In atom are 12 Sc atoms at approximately 3·20 Å. The Sc atom is surrounded by 4 In atoms at approximately 3·20 Å and 8 Sc atoms at about 3·20 Å.

The authors wish to express their sincere thanks to E. A. Wood for many helpful discussions and R. G. Treuting for the use of his IBM 7090 program for the intensity calculations.

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Acta Cryst. (1962). **15**, 94

Unit cell and space group of mercury tellurate, Hg_3TeO_6.

By Olav H. J. Christie, *Mineralogisk-Geologisk Museum, Oslo, Norway*

(*Received* 9 *October* 1961)

Because of its cubic symmetry and its large unit cell mercury tellurate is well suited as an internal standard material for high accuracy X-ray powder analysis. It may be prepared according to Hutchins (1905) by reaction between concentrated aqueous solutions of potassium tellurate and mercury nitrate in a weakly acid solution.

Table 1. *Interplanar spacings for* Hg_3TeO_6

Preparation according to Hutchins (1905). Reflections marked by a cross are also given by Westman & Magnéli (1957)

hkl	d_c	d_o	
220	4·73 Å	4·73 Å	*vw*
310	4·24	4·24	*vw*
311	4·05	4·05	*w*
320	3·72	3·72	*vw*
321	3·58+	3·58	*s*
400	3·35+	3·35	*m*
410 322	3·25	3·25	*vw*
411 330	3·16+	3·16	*vs*
331	3·07	3·06	*vw*
420	3·00+	3·00	*vs*
332	2·86	2·86	*w*
422	2·73+	2·73	*vs*
510 431	2·63	2·65	*vw*
521	2·45+	2·45	*m*
440	2·37	2·37	*vw*
530 433	2·30+	2·29	*m*
610	2·20	2·20	*w*
611 532	2·18+	2·17	*m*

The white precipitate should be kept at 80 °C. for several weeks to ensure complete recrystallization. The recrystallized product contains coarse and strongly yellow crystals of mercury tellurate that may be selected by hand.

According to Westman & Magnéli (1957) mercury tellurate is cubic ($a_0 = 13{\cdot}3921 \pm 0{\cdot}0013$ Å) and the reflections found by them indicate that $h+k+l=2n$, and thus that the unit cell is body-centered. Guinier exposures of mercury tellurate prepared as mentioned above show some additional reflections indicating that the unit cell is primitive. The obtained reflections do not allow a positive determination of the space group of the investigated material, but if the absence of the 002 reflection is systematic the space group is probably $P4_132$ or $P4_332$. If the absence of 002 is accidental, the point groups 23, $m3$, $\bar{4}3m$, and $m3m$ are also possible.

The interplanar spacings of mercury tellurate are given in Table 1.

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Acta Cryst. (1962). **15**, 95

The unit cell and space group of 2,6-dimethoxy-3,5-dichloro-4-methylbenzoic acid.

By R. PATERSON and G. A. SIM, *Chemistry Department, The University, Glasgow, W. 2., Scotland*

(*Received* 23 *October* 1961)

During studies of substituted benzene derivatives (Ferguson & Sim, 1961) crystals of 2,6-dimethoxy-3,5-dichloro-4-methylbenzoic acid were examined. From oscillation, rotation and Weissenberg photographs taken with Cu$K\alpha$ radiation we have found the unit cell to be orthorhombic with dimensions

$$a = 7{\cdot}05 \pm 0{\cdot}02,\ b = 33{\cdot}1 \pm 0{\cdot}1,\ c = 20{\cdot}69 \pm 0{\cdot}07\ \text{Å}\ .$$

The systematic absences observed are those of the space group D_{2h}^{15}–$Pbca$. The measured crystal density is 1·43 g.cm.$^{-3}$, giving sixteen molecules in the unit cell. The calculated density is 1·458 g.cm.$^{-3}$.

No further work on this compound is contemplated.

Reference

FERGUSON, G. & SIM, G. A. (1961). *Proc. Chem. Soc.*, p. 162.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (A. J. C. Wilson, Department of Physics, University College, Cathays Park, Cardiff, Great Britain). As far as practicable books will be reviewed in a country different from that of publication.

The Interpretation of X-ray Diffraction Photographs.

By N. F. M. HENRY, H. LIPSON and W. A. WOOSTER. Pp. 224 with many figs. London: Macmillan. Sec. Ed. 1960. Price 63*s*.

Since the first edition was published in 1951, 'Henry, Lipson and Wooster' has established itself as an essential reference book on the library shelves, or more often on the desks, of a majority of X-ray crystallographers. Its value for the practical man, as well as for teaching purposes, has been universally recognized. The advent of a second edition is therefore to be very warmly welcomed. Not only will it enable many more individuals to become familiar with the details of its excellently written text, but it will also make it possible to replace those copies which are suffering the consequences of continuous use over a period of nine years.

One notable feature of the present edition is that several major revisions have been effected, in order to incorporate new matter, without changing the overall length of the text appreciably. Indeed the text finishes on page 224 as it did in the original edition. This has been managed partly by transferring some items, including tables, which were previously included in the body of the book, to appendices, but also by adding paragraphs about recent developments towards the ends of chapters.

The publication during the last ten years of several other text books on particular crystallographic topics has