The structure of TiCl$_2$.* By N. C. Baenziger and R. E. Rundle. The Institute for Atomic Research of Iowa State College, Ames, Iowa, U.S.A.

An investigation of the dihalides of titanium, vanadium and chromium has been reported by Klemm & Grimm (1942) in which they were unable to determine the crystal structure of TiCl$_2$. Those investigators stated that it was not isostructural with TiI$_2$ which was found to have the CdI$_2$ (C6) type structure.

H. Lipkind has prepared TiCl$_2$ in this laboratory by the reduction of TiCl$_4$ with hydrogen in a heated quartz tube. The X-ray diffraction powder diagrams of this material can be interpreted with a hexagonal unit cell, $a = 3.561 \pm 0.005$ A., $c = 5.875 \pm 0.008$ A. The calculated X-ray density, with one TiCl$_2$ per unit cell, is 3.06 g.cm.$^{-3}$ This is in fair agreement with the value 3.13 g.cm.$^{-3}$ obtained by Klemm & Grimm by the pycnometer method. (There is a possibility that Klemm & Grimm did not have the same material.)

The intensities of the maxima have been calculated on the basis of the CdI$_2$ structure with

1 Ti at 0, 0, 0;
2 Cl at $\pm\frac{1}{3}$, $\frac{2}{3}$, u, with $u = \frac{1}{4}$.

The calculated and observed intensities are listed in Table 1. Varying the u parameter from $\frac{1}{4}$ did not improve the intensity agreement.

It seems clear from the agreement between the calculated and observed intensities that TiCl$_2$ has the CdI$_2$ structure. The diffraction data of Klemm & Grimm, which do not agree with the above, may be evidence for another crystal form.

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The intensities were calculated using $I \propto FF^*LPMA$, where F is the structure factor; F^* its complex conjugate; L and P the Lorentz and polarization factors; M the multiplicity factor; and A the absorption factor. An artificial temperature factor obtained by plotting

Table 1. *Intensity comparisons for* TiCl$_2$

Indices	Intensities Calc.	Intensities Obs.	Indices	Intensities Calc.	Intensities Obs.
00*1	51	66	20*2	21	21
10*0	2·7	—	10*4	0·3	—
00*2	5·3	15	11*3	5·4	9
10*1	260	264	20*3	9·2	15
10*2	149	110	00*5	0·4	—
11*0	80	77	21*0	0·1	—
11*1	21	17	21*1	13	18
10*3	50	50	11*4	14	18
20*0	0·5	—	10*5	4·9	9
11*2	3·5	—	21*2	10	13
20*1	30	24	20*4	0·05	—
00*4	11	11	30*0	3·9	9

$\log I_{\text{obs.}}/I_{\text{calc.}}$ versus $\sin^2\theta$ was used to bring the data into agreement over the whole range of the film. The intensities were estimated visually by comparison with standard intensity films. The lattice constants are given in true A. units; for the wave length of Cu $K\alpha$ radiation we have used 1·5418 A. (Bragg & Wood, 1947).

References

Bragg, W. L. & Wood, R. A. (1947). J. Amer. Chem. Soc. 69, 2919.

Klemm, W. & Grimm, L. (1942). Z. anorg. Chem. 249, 198.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Forthcoming publications

Messrs G. Bell and Sons Ltd., London, England, announce the forthcoming publication of the following works of crystallographic interest:

The Optical Principles of the Diffraction of X-rays. By R. W. James, being vol. II of *The Crystalline State.* Probable price 80s.

Outline of Contents: The Geometrical Theory of Diffraction by Space-lattices; The Intensity of Reflection of X-rays by Crystals; The Atomic Scattering Factor; The Anomalous Scattering and Dispersion of X-rays; The Influence of Temperature on the Diffraction of X-rays by Crystals; Experimental Tests of the Intensity Formulae; The Use of Fourier Series in Crystal Analysis; Laue's Development of the Dynamical Theory—Kossel

Lines; The Scattering of X-rays by Gases, Liquids and Amorphous Solids; Diffraction by Small Crystals and its Relationship to Diffraction by Amorphous Matter.

Crystals and X-rays. By Kathleen Lonsdale. Price about 15s.

Outline of Contents: Historical Introduction; Generation and Properties of X-rays; The Geometry of Crystals; X-ray Methods of Investigation; Geometrical Structure Determination; Determination of Atomic and Electronic Distribution; Extra-Structural Studies; The Importance of the Study of Crystals.

Messrs Bell also announce the reprinting of *The Crystalline State*, vol. I, by Sir Lawrence Bragg, and that H. Lipson has in preparation a work on *The Technique of X-ray Analysis* which will probably constitute vol. III of *The Crystalline State.*