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Neutron-diffraction study of Al_2Th.

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The following structure has been suggested for Al_2Th on the X-ray powder-pattern evidence (Braun & van Vucht, 1955):

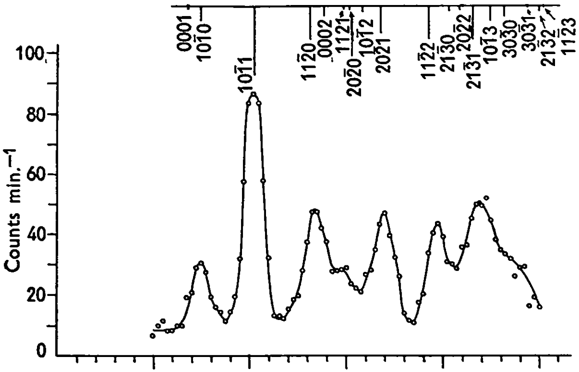

Fig. 1. Neutron-diffraction pattern of Al_2Th, with calculated intensities indicated.

Hexagonal, $a = 4.393$ Å, $c = 4.164$ Å;
Th at $(0, 0, 0)$; Al at $\pm(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$.

However, the X-ray scattering is dominated by the Th atom, and so is rather insensitive to the Al position. The neutron-scattering amplitudes are more favourable in this respect (Th = 1·01, Al = 0.35×10^{-12} cm.), and therefore the neutron powder diagram was taken as a further check.

11 g. of the alloy were used in a cylindrical specimen container of 1 cm. diameter made of aluminium. Counts were taken at intervals of 0·5° in 2θ over 20 min. The wavelength was 1·00 Å.

Good agreement was obtained between the observed intensities and those calculated for the suggested structure. This is illustrated by Fig. 1.

Reference

Braun, P. B. & Vucht, J. H. N. van (1955). *Acta Cryst.* **8**, 117.

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The crystal structure of copper hydride.

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Introduction

If solutions of hypophosphorous acid and copper sulphate are warmed together, a brown solid precipitates which gives off hydrogen when heated above 60° C. Its main constituent is believed to be copper hydride, CuH, although one can find doubt expressed as to whether this exists as a well-defined compound.

Hüttig & Brodkorb (1926) took an X-ray diagram of the precipitate from which they concluded that in the hydride the copper atoms form a face-centred cubic lattice, $a = 4.33$ Å, although they admit that this interpretation accounts for only part of the lines they observed. In what appears to be a much more careful study, Müller & Bradley (1926) conclude that the unit cell is hexagonal, $a = 2.89$, $c = 4.61$ Å, with Cu at $0, 0, 0$; $\frac{1}{3}, \frac{2}{3}, \frac{1}{2}$.

Nevertheless, some recent compilations, such as Sidgwick (1950), and also the ASTM card index, give the cubic structure. Wyckoff (1951), on the other hand, follows Müller & Bradley, and tentatively assigns the wurtzite (zincite) structure to the compound.

In view of this discrepancy, and the still somewhat dubious nature of the precipitate, we have taken up the problem once more, but now also used neutrons to verify the positions of the hydrogen atoms. Because of the large incoherent neutron scattering cross-section of hydrogen, we also prepared and investigated the deuteride.

Preparation of samples

Copper hydride was made according to Vanino (1926). The deuteride was prepared in an analogous way, using deutero-hypophosphorous acid, made from its calcium salt, which was synthesized from CaO, heavy water and white phosphorus. No attempt was made to remove all water as the precipitate becomes pyrophoric when completely dry.

X-ray analysis showed that the precipitates made in this way always contained some metallic copper, and sometimes also Cu_2O. The amounts of these impurities could be estimated from the X-ray diagrams. This, together with an electrolytic determination of the total copper content, gave the amount of water. The composition of the samples, taking total Cu as unity, was as follows:

	CuH(CuD)	Cu	Cu_2O	$H_2O(D_2O)$
Copper hydride	0·89	0·06	0·05	0·73
Copper deuteride	0·91	0·09	0·00	1·01

X-ray work

A diffractometer study of the hydride completely confirmed the results of Müller & Bradley. It was noted that the line broadening they reported is particularly pronounced for high values of l. In fact, using Jones's