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On the crystal structure of $SrB_2O_4.4H_2O$.

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$SrB_2O_4.4H_2O$ forms colourless needles. Multiple-film Weissenberg photographs were taken with unfiltered Cu radiation from crystals prepared in the Institut für anorganische und anorganisch-technische Chemie der Technischen Universität Dresden (Lehmann & Jäger, 1963).

Crystal data

Space group: $P2_1/c$.
Cell dimensions:

$a = 8{\cdot}20$ (needle axis), $b = 16{\cdot}07$, $c = 10{\cdot}91$ Å;
$\beta = 118{\cdot}5°$.

Measured density: 2·58 g.cm^{-3} at 25 °C.
Number of molecules per unit cell: $Z = 8$.

In addition to the systematic absences corresponding to the space group, systematically weak reflexions were observed for all $F(hkl)$ with $h = 2n$, $k = 4n+2$ and $h = 2n+1$, $k = 4n$. This is most probably caused by the fact that all atoms occur in pairs of the same sort, related to each other by a vector with the approximate components $(\frac{1}{2}, \frac{1}{4}, 0)$.

The following positions were obtained for the independent Sr atoms:

	x	y	z
Sr(1)	0,476	0,098	0,216
Sr(2)	−0,012	−0,156	0,214

Reference

LEHMANN, H. A. & JÄGER, H. (1963). *Z. anorg. Chem.* **326**, 31.

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The crystal structure of NbAs (comments).

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A determination of the crystal structure of NbAs has been reported rather recently by Boller & Parthé (1963). An independent investigation has been carried out in Oslo*. Although we have withdrawn our original manuscript some comments seem to be appropriate.

Samples were prepared from spectrographically standardized niobium (Johnson, Matthey & Co., Ltd.) and high purity arsenic (American Smelting and Refining Co.). A series of samples was prepared by heating accurately weighed quantities of the components (in different compositions) in evacuated and sealed silica tubes. The samples were heated at various temperatures between 720 and 1350 °C and quenched in ice water. Certain difficulties in the preparation of the samples resulted from reaction between niobium and the silica (Furuseth & Kjekshus, 1964). Samples of the NbAs phase were therefore also made by thermal decomposition of $NbAs_2$. After complete degradation at 1100 °C the residual crystalline phase was found to contain only the NbAs phase.

Guinier photographs (taken with strictly monochromatized Cu $K\alpha_1$ radiation, $\lambda = 1{\cdot}54050$ Å, with potassium chloride, $a = 6{\cdot}2919$ Å (Hambling, 1953) added as internal standard) could be indexed on tetragonal axes;

$$a = 3{\cdot}4517,\ c = 11{\cdot}680 \text{ Å},\ c/a = 3{\cdot}3838$$

in excellent agreement with the values

$$a = 3{\cdot}45_2,\ c = 11{\cdot}67_9 \text{ Å},\ c/a = 3{\cdot}38_4$$

reported by Boller & Parthé (1963). As the lattice constants are almost invariable for specimens with different initial proportions of the components, no composition range of the NbAs phase is indicated.

The composition NbAs was ascertained by density measurements. On the basis of the pycnometric density 7·93 g.cm^{-3} (at 25·00 °C), the unit cell contains 4 NbAs groups ($Z_c = 3{\cdot}96$).

The systematic extinctions were of the same type as those reported by Boller & Parthé and accordingly we had the choice between the same six space groups. Our way to the solution of the crystal structure is somewhat different from theirs and some details will be described in the following text.

A tetragonal structure with similar composition, unit-cell dimensions and systematic extinctions in X-ray photographs had been reported for β-NbP by Schönberg (1954). The possibility of the compounds being isostructural was consequently investigated.

The relative intensities of the reflexions on Debye–Scherrer photographs were determined from photometer recordings of the films. (Attempts to obtain single crystals were unsuccessful.) Multiple-film photographs were used to avoid errors in the highest and weakest intensities on the photographs. Corrections for the resolution of $K\alpha_1\alpha_2$ doublets were carried out according to the method of Rae & Barker (1961). F_o^2 values were obtained by multiplication of the corrected intensities

* *Note added in proof.* — Another independent study of NbAs has been published by Saini, Calvert & Tayler (1964) since this manuscript was accepted for publication. Their lattice dimensions and observed density are:

$a = 3{\cdot}443 \pm 0{\cdot}002$, $c = 11{\cdot}672 \pm 0{\cdot}005$ Å, $D_m = 8{\cdot}11$ g.cm^{-3}.