

We measured a density of 5.25 for a solid sample with a 12:1 atomic ratio of boron to tungsten. If the composition of the boride is WB_4 , then allowing for the free boron, the density of the boride is 9.9. If the boride is WB_5 , the experimental density is 8.7. Assuming 4 formula units per hexagonal unit cell, the theoretical density is 10.16 for WB_4 and 10.64 for WB_5 , both reasonably close to 9.9.

In view of the large difference between atomic scattering factors of tungsten and boron it is very difficult to determine the locations of the boron atoms from X-ray measurements and it should be possible to calculate a first approximation of the structure factor by neglecting the contribution of the boron atoms. Partial structure factor calculations for the tungsten alone gave reasonable agreement with observed structure factors calculated from powder data when the following positions in space group $P6_3/mmc$ were used:

$$\begin{array}{ll} 2W(1) \text{ in } 2(c) & \frac{1}{3}, \frac{2}{3}, \frac{1}{4}; \frac{2}{3}, \frac{1}{3}, \frac{1}{4} \\ 2W(2) \text{ in } 2(b) & 0, 0, \frac{1}{4}; 0, 0, \frac{3}{4} \end{array}$$

The above arrangement of tungsten atoms limits the boron atoms of the following positions:

$$\begin{array}{ll} 12B(1) \text{ in } 12(i) & x, 0, 0; \text{ etc.} \\ 4B(2) \text{ in } 4(f) & \frac{1}{3}, \frac{2}{3}, z; \text{ etc.} \end{array}$$

A value of $\frac{1}{3}$ for X places the boron atoms of the first group equidistant from the surrounding tungsten atoms at a distance of 2.35 Å. Assuming a B-B distance of 1.72 Å (as in W_2B_5) for adjacent boron atoms of the second group, the

W-B distance is 2.31 Å which is the same as the shortest W-B distance in W_2B_5 . These values correspond to a z of 0.615. The distance of closest approach of two tungsten atoms is 3.00 Å compared with 2.98 Å for W_2B_5 . Intensities calculated from the above tungsten and boron positions are included in Table 2.

The proposed structure is closely related to the AlB_2 structure which consists of close packed layers of metal atoms located directly above one another with boron atoms in the interstices. The WB_4 structure can be derived from the AlB_2 structure by replacing one third of the metal atoms with pairs of boron atoms systematically so that the remaining metal atoms form layers of open hexagons with alternate layers displaced by one atom. It is possible that additional tungsten atoms might be randomly replaced by boron pairs which could account for the experimental composition we observed.

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The neutron coherent scattering amplitude of caesium. By M. S. ŽIVADINOVIĆ and B. V. PRELESNIK, *Laboratory for Solid State Physics, Boris Kidrič Institute of Nuclear Sciences, Belgrade, Yugoslavia*

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The neutron coherent scattering amplitude of the caesium atom, equal to 0.49×10^{-12} cm according to *International Tables for X-Ray Crystallography* (1962), was used in neutron diffraction investigations of the crystal structure of caesium uranyl nitrate*. The positions of heavy atoms in this structure, including caesium, are known from the X-ray study of Malčić & Manojlović (1961). However, the difference Fourier syntheses applied in our refinement showed the presence of high positive peaks in the caesium atom position. Assuming the work of Malčić & Manojlović to be correct, this suggests that the value taken for the neutron scattering amplitude of caesium is probably too low. To solve the problem, we have reinvestigated this constant.

The neutron diffraction measurements were made on a powder sample of CsCl, Merck's product of a quality normally used in preparing crystals for structure analysis. The sample was contained in a 5 cm long vanadium tube of 0.1 mm wall thickness and 10 mm diameter. The powder diagrams were recorded on a neutron diffractometer on the nuclear reactor RA of this Institute. The neutron wavelength was 1.031 Å. The intensities were brought to an absolute scale by scaling from a nickel powder diagram, obtained under the same experimental conditions.

* To be published elsewhere.

The powder diagram of CsCl is shown in Fig. 1. The accuracy of the diffraction peak areas was estimated to 3% or better. The absorption correction was made, and the experimentally determined value of μR for CsCl was found to be 0.17 cm^{-1} and $q'/q_0 = 0.645$.

The scattering amplitude of caesium was calculated following the method described by Shull & Wollan (1951) and Sidhu, Heaton & Mueller (1959). The integrated intensities of the reflexions with $h+k+l=2n$ were used. The numerical value of the experimental constant K was obtained from the nickel sample, the scattering amplitude being 1.03×10^{-12} cm. The plot of F_{hkl} observed versus $(\sin \theta)^2/\lambda^2$, for nickel and $h+k+l=2n$ reflexions of CsCl, is shown in Fig. 2. The value of $F(0)_{hkl}$ for CsCl as determined by least squares is found to be 1.742×10^{-12} cm. From the expression $F(0) = bc_s + bc_l$ for the $h+k+l=2n$ reflexions and the known value of the scattering amplitude of chlorine, equal to 0.99×10^{-12} cm, as given in *International Tables for X-Ray Crystallography* (1962), we found the coherent scattering amplitude of caesium to be $(0.75 \pm 0.02) \times 10^{-12}$ cm.

The values of the coherent scattering amplitude of caesium and rubidium quoted in *International Tables for X-Ray Crystallography* (1962) were determined by Shull & Wollan (1951). Our value of bc_s is considerably higher than the previously reported one of 0.49×10^{-12} cm. The recently

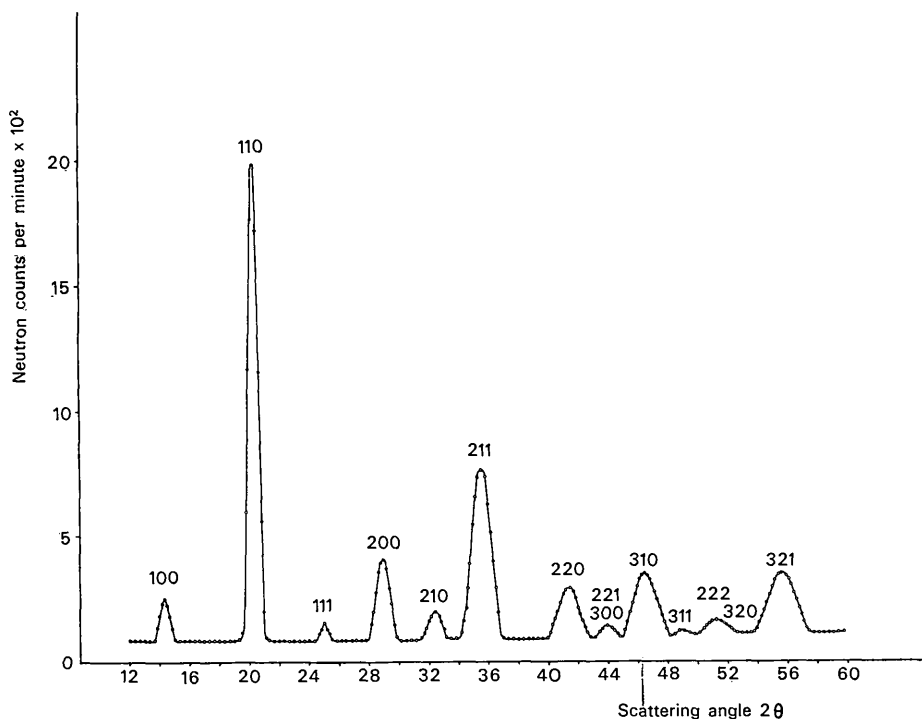


Fig. 1. Neutron diffraction powder diagram of caesium chloride, $\lambda = 1.031 \text{ \AA}$.

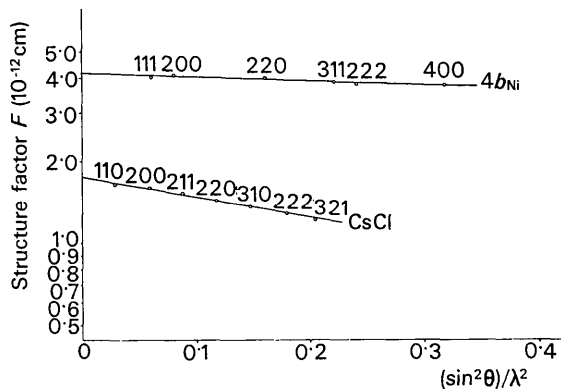


Fig. 2. Structure factors of nickel and caesium chloride as the functions of $(\sin^2 \theta)/\lambda^2$.

redetermined b_{Rb} of $0.85 \times 10^{-12} \text{ cm}$ by Mueller, Sidhu, Heaton, Hitterman & Knott (1963) is also considerably higher than the previous one of $0.55 \times 10^{-12} \text{ cm}$. It is interesting to note that the redetermined constants both for caesium and rubidium are, therefore, higher by a factor of about 1.5 than the previous ones.

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Transformation of thermal vibration tensors. By C. SCHERINGER, *Institut für Kristallographie der Technischen Hochschule Aachen, Germany*

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It has been found that the formulae for the transformation of thermal vibration tensors given by Cruickshank (1956a, 1961) have to be modified for oblique crystal systems, and thus also the programs based on them. The appropriate formulae will be derived. The mathematical formalism used is also chosen to allow a comparison between the existing methods of determining the principal representation of the vibration tensors, and to derive an explicit formula for

their symmetry-equivalent representations. We refer to Cruickshank's papers as CR and CRU respectively. If not stated otherwise, the notation will be as used in CR.

Transformation in oblique crystal systems

CR equation (1.6) for the 'smearing function' $t(\mathbf{X})$ and CR equation (1.7) for its transform $q(\mathbf{S})$ are only valid for or-