Short Communications

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A redetermination of the coherent neutron scattering amplitude of rubidium.

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The coherent neutron scattering amplitude of rubidium has been remeasured using powders of RbCl, RbBr, and RbI. A consistent value, $(0{\cdot}68_5 \pm 0{\cdot}01) \times 10^{-12}$ cm, was obtained, differing significantly from earlier measurements. The new value is believed to be more reliable. The bound coherent scattering cross-section is $5{\cdot}9 \pm 0{\cdot}2$ barns.

The coherent neutron scattering amplitude of rubidium (b_{Rb}) was first measured by Shull & Wollan (1951) who obtained $b_{Rb} = 0{\cdot}55$ (scattering amplitudes are given throughout in units of 10^{-12} cm). In their structure study of $RbMnF_3$, Pickart, Alperin & Nathans (1964) found this value low, and favoured a value of about 0·63. Mueller, Sidhu, Heaton, Hitterman & Knott (1963) reported a value of 0·85. In view of the considerable discrepancy between these measurements, a further investigation has been undertaken in order to obtain a better value of b_{Rb}.

The previously published values were both obtained by the powder diffraction technique (Bacon, 1962) using samples of RbCl and an external standard. The present measurements were made by the powder method using cylindrical samples of RbCl, RbBr, and RbI (which have the NaCl structure) using the halogens as internal standards. For cylindrical geometry and the NaCl structure, the integrated intensity, P, of the reflexion from a set of planes (hkl) is $P = KjI/(\sin\theta \sin 2\theta)$ where

$$I = |b_{Rb} \exp(-W_{Rb}) \pm b_X \exp(-W_X)|^2 A .$$

Here j is the multiplicity of the (hkl) planes, θ is the Bragg scattering angle, b_X is the coherent scattering amplitude of the halogen, the exponential terms are Debye–Waller temperature factors, and A is the absorption factor: P, I, j, θ, W_{Rb}, W_X, and A depend on the indices hkl. K is a constant depending on details of the spectrometer and on the size of the sample. The plus (minus) sign is used when h, k, l are all even (all odd). In this work, the intensities of the 111 and 200 reflexions from each halide were measured and a consistent value of b_{Rb} was obtained from the intensity ratios P_{111}/P_{200}.

Measurements were made at room temperature using the McMaster University triple-axis spectrometer at Chalk River (Brockhouse, de Wit, Hallman & Rowe, 1968) with $\lambda = 1{\cdot}335$ Å. The analyser was set to count neutrons elastically scattered by the specimen. Use of a double monochromator and an analyser significantly reduces second order contributions to the measured intensities. The specimens (obtained from K & K Laboratories, Plainsview, New York, 99·9% pure), were contained in a half inch diameter aluminum can having 0·012 inch walls.

The ratios $R_X = I_{111}/I_{200}$, are given in Table 1. The 111 peak in RbBr was too weak to be seen. The errors assigned to the ratios R_X arise from counting statistics. Neglecting the absorption and temperature factors we may write $R_X = (b_{Rb} - b_X)^2/(b_{Rb} + b_X)^2$. Since R_{Br} is very small, $b_{Rb} \simeq b_{Br}$. The values of b_{Rb} listed in Table 1 were obtained

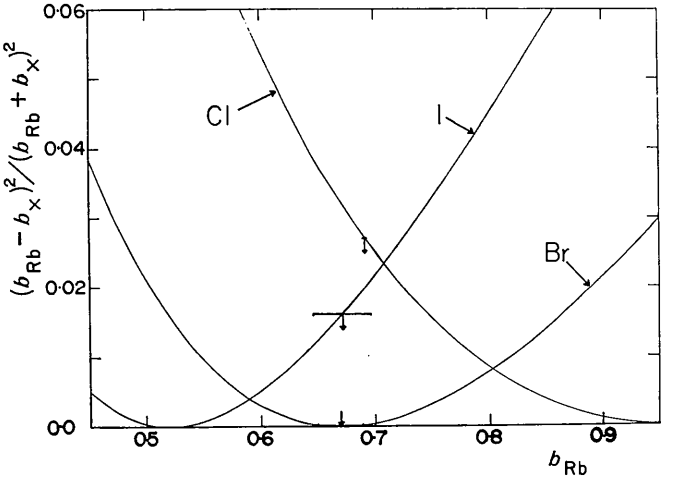

Fig. 1. The ratio $(b_{Rb} - b_X)^2/(b_{Rb} + b_X)^2$ as a function of b_{Rb}, for the three halogens. The arrows indicate the values of b_{Rb} deduced from each intensity ratio, neglecting temperature corrections. The short horizontal lines represent uncertainties in b_{Rb} arising from uncertainties in the values of b_X.

from the ratios R_X, corrected for the temperature factors as described below. The values of b_X are also given in Table 1. Fig. 1 illustrates the dependence of b_{Rb} on the ratios R_X.

Table 1. *Powder diffraction results from several* Rb *halides*

$R_X = I_{111}/I_{200}$ is calculated from the observed intensities; b_X is the assumed halogen scattering amplitude, and b_{Rb} is the calculated scattering amplitude for Rb. Scattering amplitudes in units of 10^{-12} cm.

X	Cl	Br	I
R_X	$0{\cdot}027_2 \pm 0{\cdot}001$	$0{\cdot}0 \pm 0{\cdot}0002$	$0{\cdot}016_4 \pm 0{\cdot}001$
b_X	$0{\cdot}963 \pm 0{\cdot}001$*	$0{\cdot}67 \pm 0{\cdot}02$†	$0{\cdot}52 \pm 0{\cdot}02$†
b_{Rb}	$0{\cdot}69 \pm 0{\cdot}01$	$0{\cdot}67 \pm 0{\cdot}02_5$	$0{\cdot}67 \pm 0{\cdot}03$

* Koester (1967).
† Shull & Wollan (1951).

Individual room temperature Debye–Waller parameters, $B_i = W_{i,hkl}(\lambda/\sin\theta_{hkl})^2$ were calculated (Dolling, Smith, Nicklow, Vijayaraghavan & Wilkinson, 1968) using the breathing shell model (Schröder, 1966) with the elastic and optical constants as input parameters. In the worst case, that of RbI, inclusion of the temperature factors reduces the calculated value of b_{Rb} by $(0{\cdot}7 \pm 0{\cdot}7)\%$ to the value given. The average Debye–Waller parameter for RbI, obtained from the relative intensities of 8 even *hkl* reflexions, was 3·6 Å^2, in substantial agreement with calculated values of 3·4 and 3·6 (5) Å^2, for the Rb^+ and I^- ions respectively. The degree of contamination of the monochromatic beam is best estimated from the ratio R_{Br}, since the 1st order 111 reflexion also contains a 2nd order 222 contribution. On this basis, corrections to b_{Rb} are estimated to be $<0{\cdot}1\%$. Absorption corrections are $<0{\cdot}01\%$.

From the 3 independent measurements of b_{Rb}, we obtain a best value, $b_{Rb} = 0{\cdot}68_5 \pm 0{\cdot}01$. The bound coherent scattering cross-section, $4\pi b_{Rb}^2$, is $5{\cdot}9 \pm 0{\cdot}2$ barns. This work is in agreement with recent measurements of Wang & Cox (1970), who obtain $b_{Rb} = 0{\cdot}70_5 \pm 0{\cdot}02_5$ from the intensities of 18 reflexions in a powder sample of RbCl. Mueller *et al.* (1963) obtained $b_{Rb} = 0{\cdot}85$ using an external nickel standard. In that experiment an intensity ratio $I_{111}/I_{200} = 0{\cdot}030$ was obtained (Mueller, 1969), which gives $b_{Rb} \simeq 0{\cdot}68$. However the 111 and 200 reflexions were not fully resolved. These considerations indicate that the present measurements are more reliable than the earlier work.

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The coherent neutron scattering amplitude of Rb: a neutron diffraction study of RbCl.*

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The coherent neutron scattering amplitude of Rb has been determined by a least-squares refinement of diffraction data from RbCl. The value obtained was $0{\cdot}70_5 \pm 0{\cdot}02_5 \times 10^{-12}$ cm, which differs considerably from values previously reported in the literature.

Recent magnetic and optical measurements on mixed alkali metal-transition metal halides of perovskite type ABX_3 have revealed a number of interesting properties. Among these halides the rubidium compounds $RbFeF_3$ and $RbMnF_3$ have been studied in considerable detail *e.g.* Wang & Kestigian (1966), Wertheim, Guggenheim, Williams & Buchanan (1967), Testardi, Levinstein & Guggenheim (1967), Corliss, Delapalme, Hastings, Lau & Nathans (1969). During the course of a neutron diffraction study of $RbFeF_3$ (Wang, Cox & Kestigian, 1968) it was found that the coherent neutron scattering amplitude value for Rb of $0{\cdot}85 \times 10^{-12}$cm determined by Mueller, Sidhu, Heaton, Hitterman & Knott (1963), and listed in the recent Neutron Diffraction Commission (1969) compilation, could not account for the observed nuclear intensity data. In addition to this value, widely different values of $0{\cdot}55 \times 10^{-12}$ cm (Shull & Wollan, 1965) and $0{\cdot}63 \times 10^{-12}$ cm (Pickart, Alperin & Nathans, 1964) have also been reported. A

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