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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† Guest scientist at Brookhaven National Laboratory.

least-squares refinement of data from a rather impure polycrystalline sample of $RbFeF_3$ in the above-mentioned neutron diffraction study yielded a value of $0{\cdot}67 \times 10^{-12}$cm (almost exactly the mean of the three reported values!).

In order to obtain a reliable value for $b_{\rm Rb}$, a neutron diffraction study of RbCl was undertaken. There are very few compounds of Rb suitable as standards of this sort, and RbCl is probably the most satisfactory, as it is readily available in a pure state and has a simple rock-salt type structure. In addition, $b_{\rm Cl}$, relative to which $b_{\rm Rb}$ is determined, is known with considerable accuracy. A polycrystalline sample of Johnson Matthey 'Specpure' material was used. This was dried at 400 °C in a chlorine atmosphere, transferred to a glove box to exclude moisture, and loaded into an aluminum sample holder ⅜ inch in diameter and 3 inches long. Neutron diffraction data were obtained at 25 °C at the Brookhaven High Flux Beam Reactor facility. A neutron beam of wavelength 1·034 Å from the 311 reflection of a germanium monochromator was utilized. Since the 622 reflection is absent, second-order wavelength contamination is therefore eliminated, while third-order contamination is found to be negligible.

The diffraction pattern showed a total of 21 resolvable peaks, of which three overlapped with Al peaks from the sample holder. Six reflections were of the type with h, k, and l all odd. These have structure factors proportional to $b_{\rm Rb} - b_{\rm Cl}$ and are very weak. Since $b_{\rm Rb}$ depends sensitively upon the intensities of peaks of this sort, it is important that these be measured as accurately as possible. The absence of halfwavelength contamination is clearly very advantageous in this respect.

A least-squares refinement of 18 peaks based upon intensities was made with a program which allows overlapping reflections to be used (Hamilton, 1962). No corrections were made for absorption, which is negligibly small, while extinction effects were assumed to be absent. The coherent scattering amplitude of Cl was taken as $0{\cdot}963 \times 10^{-12}$cm (Koester, 1967). In addition to $b_{\rm Rb}$, individual isotropic temperature factors $B_{\rm Rb}$ and $B_{\rm Cl}$ were treated as variable parameters. The final values obtained are listed in Table 1. Corresponding observed and calculated intensities are shown in Table 2.

Table 1. *Parameter values from least-squares refinement of neutron powder data from* RbCl

Standard errors are given in parentheses.

$b_{\rm Rb}$	0·704 (10) × 10^{-12} cm
$B_{\rm Rb}$	2·2 (2) Å^2
$B_{\rm Cl}$	2·3 (1) Å^2
R factor	5·2%
Weighted R factor	7·2%

Table 2. *Comparison of observed and calculated intensities for* RbCl

Space group $Fm3m$; Rb in 4(a) at 0,0,0; Cl in 4(b) at ½,½,½. Parameters as in Table 1.

hkl	$I_{\rm calc}$		$I_{\rm obs}$
111	13·4		13·2
200	308·3		319·1
220	overlap with Al		
311	8·8		10·2
222	114·4		102·8
400	58·8		62·5
331	4·1		7·0
420	172·0		178·8
422	131·1		127·8
511	2·3	3·1	2·9
333	0·8		
440	overlap with Al		
531	2·9		2·7
600	16·8	84·0	86·7
442	67·2		
620	55·3		57·2
533	1·0	46·6	47·6
622	45·6		
444	12·9		9·0
711	0·7	34·3	37·2
551	0·7		
640	32·9		
642	56·0		60·3
731	1·0	1·5	1·2
553	0·5		
800	overlap with Al		
733	0·3	36·3	33·3
820	18·0		
644	18·0		

As is usually the case in a refinement of this sort, there were appreciable correlation effects between the scattering amplitude, temperature factor and scale factor. Significance tests on $b_{\rm Rb}$ were therefore carried out according to the procedure described by Hamilton (1965). The confidence intervals at the 95% and 99% levels were found to be about ±0·02 and $\pm 0{\cdot}03 \times 10^{-12}$cm respectively, and the final value of $b_{\rm Rb}$ has therefore been chosen as $0{\cdot}70_5 \pm 0{\cdot}02_5 \times 10^{-12}$cm.

The isotropic temperature factors listed in Table 1 are in excellent agreement with values of 2·28±0·10 and 2·44±0·10Å^2 for $B_{\rm Rb}$ and $B_{\rm Cl}$ respectively reported in a recent X-ray diffraction study by Järvinen & Inkinen (1967). From the values in Table 1, Debye temperatures of 137 and 210 °K were calculated for Rb and Cl respectively. These may be compared with the published value of 162 °K for RbCl found from elastic measurements (Fedorov, 1968).

The scattering amplitude of Rb has also been determined in a recent study by Copley (1970) of RbCl, RbBr, and RbI. He obtains a value of $0{\cdot}68_5 \pm 0{\cdot}01 \times 10^{-12}$cm, in good agreement with the result presented here.

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Errata in *International Tables for X-ray Crystallography*, Vol. I (2nd edition).

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(*Received* 8 *October* 1969)

A corrected electron density expression is given for space groups $P4_122$ (No. 91) and $P4_322$ (No. 95).

The electron density expressions for the enantiomorphous space groups $P4_122$ (No. 91, p. 426) and $P4_322$ (No. 95, p. 429) should read:

$$\varrho(XYZ) = \frac{8}{V_c}\left\{\sum_0^\infty \sum_0^\infty \sum_0^\infty {}^{l=2n} |F(hkl)| \, [\cos 2\pi hX \times \cos 2\pi kY \cos 2\pi lZ \cos \alpha(hkl) - \sin 2\pi hX \sin 2\pi kY \sin 2\pi lZ \sin \alpha(hkl)] + \sum_0^\infty \sum_0^\infty \sum_0^\infty {}^{l=2n+1} |F(hkl)| \, [-\sin 2\pi hX \times \cos 2\pi kY \sin 2\pi lZ \cos \alpha(hkl) + \cos 2\pi hX \sin 2\pi kY \cos 2\pi lZ \sin \alpha(hkl)]\right\}.$$

Corrections to the phase relationships have appeared already (Schultze-Rhonhof, 1966).

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The structure of Mn_2Au and Mn_3Au.

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(*Received* 8 *December* 1969)

X-ray and neutron diffraction measurements have shown that Mn_2Au is a compound with a tetragonal unit-cell of dimensions $a = 3{\cdot}328$ and $c = 8{\cdot}539$ Å and that it can be assigned to the same space group as $MnAu_2$, namely $I4/mmm$ (D_{4h}^{17}). The neutron diffraction pattern of 74·2 at.% MnAu can be explained only if the ordered structure of this alloy is identical with that of Mn_2Au. Thus the compound Mn_3Au apparently does not exist.

Introduction

In their investigation of the phase diagram of the Mn–Au system, Raub, Zwicker & Baur (1953) proposed the existence of the compound Mn_3Au, and from X-ray diffraction of a 70 at. % Mn alloy they concluded that it had a complex tetragonal structure, and also remarked on the similarity of the diffraction pattern to that obtained from an alloy of composition Mn_2Au.

Gaunt & Eden (1965) proposed a tetragonal structure for Mn_3Au with cell dimensions $a = 4{\cdot}706$, $c = 8{\cdot}539$ Å and atomic coordinates

Au: $000;\ \tfrac{1}{2}0\tfrac{1}{2};\ 0\tfrac{1}{2}\tfrac{1}{2};$
Mn: $00 \pm z;\ \tfrac{1}{2}0\tfrac{1}{2} \pm z;\ 0\tfrac{1}{2}\tfrac{1}{2} \pm z$
$\tfrac{1}{2}\tfrac{1}{2} \pm z;\ \tfrac{1}{2}\tfrac{1}{2}0$

with $z \simeq \tfrac{1}{3}$.

They also commented on the close similarity of this structure to that determined for $MnAu_2$ by Hall & Royan (1959).

During an investigation of Mn_3Au it was found that the neutron diffraction patterns could not be explained in terms of the above structure, and this prompted the following study.

Experimental

Three ingots, each weighing about 60g, were prepared by melting together manganese (4*N*5) and gold (5*N*) in an argon arc furnace. The ingots were homogenized at 900°C *in vacuo* for 50 hours and annealed at 500°C for a further 50 hours. Chemical analysis showed the compositions of the ingots to be 62·6, 67·4 and 74·2 at. % Mn.

X-ray diffraction patterns from flat polished specimens of all three compositions were similar to that reported by