Levy & Peterson, 1957) placed the hydrogen atoms directly in the plane of the urea molecule, and the X-ray analysis of triaminoguanidinium chloride gave a similar result.

All the hydrogen atoms in this structure are off the nitrogen–chloride line of their respective nitrogen atoms. The average hydrogen–nitrogen–chloride angle is 15·0°; the individual angles are given in Table 4.

The two coplanar guanidinium ions that coordinate the chloride ion form a structural feature that is similar to the planes of guanidinium chloride perpendicular to the *a* axis found in the guanidinium chloride–*N*,*N*-dimethylacetamide complex. These planes of guanidinium chloride are held together by additional guanidinium chloride molecules acting as cross-ties. The coordination number of the chloride ion is nearly the same in both structures.

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References

BRYDEN, J. H. (1957). *Acta Cryst.* **10**, 677.
GELLER, S. & BOOTH, D. P. (1958). *Z. Kristallogr.* **111**, 117.
HAAS, D. J., HARRIS, D. R. & MILLS, H. H. (1965. *Acta Cryst.* **18**, 623.
International Tables for X-ray Crystallography (1952) Vol. I. Birmingham: Kynoch Press.
OKAYA, Y. & PEPINSKY, R. (1957). *Acta Cryst.* **10**, 681.
THEILACKER, W. (1931). *Z. Kristallogr.* (A), **76**, 203.
THEILACKER, W. (1935). *Z. Kristallogr.* (A), **90**, 51, 256.
WORSHAM, J. E., LEVY, H. A. & PETERSON, S. W. (1957). *Acta Cryst.* **10**, 319.

Short Communications

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The scattering length of yttrium for thermal neutrons.

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The scattering length of yttrium, b_Y, for thermal neutrons has so far been determined only from the scattering of its compounds, and the accuracy depends on the reliable knowledge of their structures. Neutron diffraction studies by powder methods on yttrium aluminum garnet, $Y_3Al_2(AlO_4)_3$, by Prince (1957), yttrium carbide, YC_2, by Atoji (1963) and yttria, Y_2O_3, by Villain (1957), Fert (1962) and Kuz'minov, Yamzin, Mal'tsev & Belov (1962) give the values listed in Table 1. The results for yttria range from $0{\cdot}71\times10^{-12}$ to $0{\cdot}816\times10^{-12}$ cm, and the extremes differ considerably from the other determinations. The yttria structure conforms to space group $Im3$, with eight metal ions at the special positions $\frac{1}{4},\frac{1}{4},\frac{1}{4}$, and the remaining twenty-four at the sites $u,0,\frac{1}{4}$. The forty-eight oxygen ions are in general positions x, y, z. The largest value of b_Y by Kuz'minov *et al.* is based on an incorrect structural model conforming to space group $I2_13$ which was originally proposed by Zachariasen (1926, 1952). This determination is therefore rather suspect, and is ignored in the subsequent discussion. Villain and Fert used the neutron diffraction powder data to make least-squares analyses in which the four independent parameters and the yttrium scattering length were used as variables. A mean isotropic temperature factor coefficient was determined from a graphical comparison of the observed and calculated structure factors in the usual manner. The atomic coordinates from these analyses are listed in Table 2. The structure of yttria has recently been refined by X-ray methods using three-dimensional data from a single crystal (Paton & Maslen, 1965). The structural parameters, which are included in Tables 2 and 3, are considerably more accurate than those reported previously. In view of this a redetermination of the yttrium scattering length is warranted.

Table 1. *Scattering length of yttrium for thermal neutrons*

Authors	b_Y (cm × 10^{-12})
Prince	0·80 ±0·01
Villain	0·71
Fert	0·79 ±0·02
Kuz'minov *et al.*	0·816±0·07
Atoji	0·786±0·017
Paton & Maslen	0·781±0·008
Best mean value	0·788±0·005

Table 2. *Atomic coordinates for the yttria structure*

Author	*u*	*x*	*y*	*z*
Villain	−0·034	0·396	0·155	0·383
Fert	−0·0314±8	0·389±2	0·150±1_5	0·377±2
Paton & Maslen	−0·0328±2	0·389±1	0·154±1	0·378±1

A neutron diffraction pattern was recorded for this purpose using the powder spectrometer at the A.A.E.C. Research Establishment at Lucas Heights, New South Wales. The monochromatic beam, which was produced by reflex-

Table 3. *Thermal parameters for the yttria structure*

The temperature factor is given by $\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{23}kl+B_{13}hl+B_{12}hk)$ except for that of Y($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$), which is isotropic, and is given by $\exp\{-(B\sin^2\theta/\lambda^2)\}$.

Atom	B	B_{11}	B_{22}	B_{33}	B_{23}	B_{13}	B_{12}
Y($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$)	0·98						
Y(u, 0, $\frac{1}{4}$)		0·0019	0·0028	0·0018	0·0000	0·0000	0·0000
O		0·0031	0·0027	0·0035	−0·0001	−0·0006	0·0017

ion from the (111) face of a copper crystal, had a mean wavelength of 1·067 Å. The powder sample which was cylindrical was held in an aluminum container, and the intensities of the diffracted beams were measured with a two-inch BF_3 proportional counter, coupled to a ratemeter and chart recorder. A relatively large sample was necessary to produce scattered beams strong enough to be measurable. Thus the lines in the neutron diffraction pattern were broad, subtending an angle of approximately one degree at the specimen, and only the low angle reflexions could be resolved.

The intensities of twelve low angle lines were measured by integrating under the intensity curve in the region of each peak, and subtracting a mean value for the background. The intensities were corrected for the Lorentz factor, giving the values listed in Table 4.

Table 4. *Neutron diffraction powder line intensities*

$h^2+k^2+l^2$	I obs. ($cm^2\times10^{-24}$)	I calc. ($cm^2\times10^{-24}$)
12	3647	4177
14	711	831
22	3332	3485
26	1342	1751
30	1310	1133
32	19359	18723
38	1594	1981
42	1626	1976
44	8195	7612
46	3553	3750
54	7311	6714
62	3537	3386

A complicating feature of the pattern was the aluminum lines from the specimen container. There was preferred orientation in the aluminum and consequently the line intensities could not be calculated from the structure. However, they were readily identified from their d-spacing and did not overlap with any of the strong yttria lines in the low angle region.

The intensities of the scattered neutron lines depend on the neutron scattering length, and the atomic coordinates and thermal vibration parameters of the atoms. The structural parameters are known from the X-ray analysis, and the neutron scattering length of oxygen has been accurately determined to be $0{\cdot}577\times10^{-12}$ cm (*International Tables for X-ray Crystallography*, 1962). The ratio of the scattering length of yttrium to that of oxygen was determined by the usual method for non-linear least squares. An initial value of b_Y was selected by evaluating the agreement index

$$R=\Sigma|I_o-I_c|/\Sigma|I_c|\,,$$

where I_o and I_c are the observed and calculated intensities, for a series of values of b_Y ranging from 0·75 to $0{\cdot}83\times10^{-12}$ cm (Fig. 1). The agreement factor reached a sharp minimum

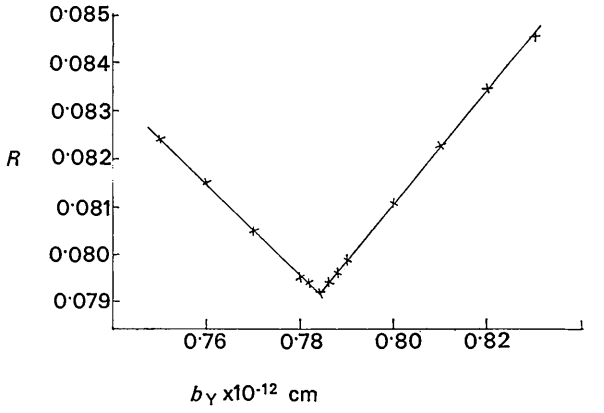

Fig. 1. Dependence of agreement residual (R) on scattering length (b_Y) of yttrium for thermal neutrons.

at $0{\cdot}784\times10^{-12}$ cm. The scale factor and b_Y were then refined through several cycles of least squares until the values were stationary, indicating that the refinement was complete. The final value was $0{\cdot}781\pm0{\cdot}008\times10^{-12}$ cm. The intensities calculated for this value of b_Y are given in Table 4. The agreement factor on these intensities is 0·077.

The result obtained does not differ significantly from those reported by Prince, Atoji and Fert, but there is a large discrepancy between these values and that of Villain, and it seems probable that this last is in error. The accuracy achieved in the present analysis is somewhat higher than in the previous determinations since there were only two variable parameters, the remainder having been determined accurately by the X-ray analysis. A still more reliable value may be derived by taking a weighted mean of the four consistent results, which gives a best value of $0{\cdot}788\pm0{\cdot}005\times10^{-12}$ cm.

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References

ATOJI, M. (1963). *J. Chem. Phys.* **35**, 1950.
FERT, A. (1962). *Bull. Soc. franç. Minér. Cryst.* **85**, 267.
International Tables for X-ray Crystallography (**1962**). Vol. I, p. 229. Birmingham: Kynoch Press.
KUZ'MINOV, YU. S., YAMZIN, I. I., MAL'TSEV, E. I. & BELOV, N. V. (1962). *Soviet Phys. Cryst.* **7**, 767.
PATON, M. G. & MASLEN, E. N. (1965). *Acta Cryst.* **19**, 307.
PRINCE, E. (1957). *Acta Cryst.* **10**, 787.
VILLAIN, J. P. (1957). Diplôme d'études supérieures, Paris.
ZACHARIASEN, W. (1926). *Norsk. Geol. Tidsskr.* **9**, 310,
ZACHARIASEN, W. (1952). *Structure Reports* **16**, 218.