

The form factor f_0 for a stationary atom is approximated by a sum of the Gaussian functions (Forsyth & Wells, 1955)

$$f_{i0} = A_{i1} \exp(-a_{i1}s^2) + A_{i2} \exp(-a_{i2}s^2) + A_{i3} \exp(-a_{i3}s^2) \quad (2)$$

with $a_{i3} = 0$, where $s = \sin \theta / \lambda$. Equation (1) is, then, easily integrated, and we obtain

$$\left. \begin{aligned} \rho_i(0) &= 8\pi^{3/2} \sum_{k=1}^3 \frac{A_{ik}}{(a_{ik} + B_i)^{3/2}} \\ P_{ij}(0) &= 8\pi^{3/2} \sum_{k=1}^3 \sum_{k'=1}^3 \frac{G_{kk'}}{(g_{kk'})^{3/2}} \end{aligned} \right\} \quad (3)$$

where

$$G_{kk'} = A_{ik}A_{jk'}, \quad g_{kk'} = a_{ik} + B_i + a_{jk'} + B_j$$

and B_i is the isotropic temperature factor of the i th atom. Although the relations (3) are not suitable at very low temperatures, they give sufficiently good approximations for most purposes. Parameters A_k and a_k in equation (2) were obtained by Moore (1963), and also by Hosoya & Satake (1965). Hosoya & Satake's parameters for the Mo range were used for calculation of the function $\rho(0)$ and the self Patterson function $P_{ii}(0)$ of various atoms. The results are shown in Table 1.

Practically, however, observed values are in general considerably smaller than these values because of termination.

In order to calculate $\rho(0)$ and $P_{ii}(0)$ subjected to the termination effect, equations (1) were rewritten as

$$\left. \begin{aligned} \rho_i(0) &= 32\pi \int_0^{1/\lambda} s^2 f_i ds \\ P_{ii}(0) &= 32\pi \int_0^{1/\lambda} s^2 f_i^2 ds \end{aligned} \right\} \quad (4)$$

Substituting relation (2) into (4), values of $\rho_i(0)$ and $P_{ii}(0)$ were obtained numerically for various wavelengths. Typical results are shown in Fig. 1. With Mo $K\alpha$, the termination is not very serious unless the temperature factor is too small, but with Cu $K\alpha$ the reduction of peak height is significant. Therefore, values for the Cu $K\alpha$ range are shown in Table 2. Tables 1 and 2 will be helpful for judging the atomic species, by reading through the column with a relevant B value.

The numerical calculations were carried out on OKITAC 5090H computer of this Institute. The author expresses his sincere thanks to Dr T. Ito of this Institute for his critical discussions.

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The crystal structure of CsUF₆*. By ABRAHAM ROSENZWEIG† and DON T. CROMER, *University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544, U.S.A.*

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CsUF₆ is rhombohedral, $a = 5.417 \text{ \AA}$, $\alpha = 95^\circ 29' 5''$, space group $R\bar{3}$, with one formula unit per unit cell. The U atom has 6F neighbors at 2.057 Å which make an octahedron slightly compressed along the threefold axis. The Cs atom has 12 neighbors, 6 at 3.101 and 6 at 3.147 Å. The compound is isostructural with KOsF₆.

The preparation of cesium uranium(V) hexafluoride was first reported by Penneman, Sturgeon & Asprey (1964), who found a rhombohedral lattice with hexagonal cell dimensions of $a = 8.036 \pm 0.003$, $c = 8.388 \pm 0.004 \text{ \AA}$. These dimensions suggest that the compound is isostructural with KOsF₆ whose structure, based on powder diffraction data, was reported by Hepworth, Jack & Westland (1956). Optical properties, cleavage and twinning were reported by Sturgeon, Penneman, Kruse & Asprey (1965). A partial absorption spectrum was reported by Asprey & Penneman (1964) and a detailed analysis of the absorption spectrum was made by Reisfeld & Crosby (1965), who assumed the centric space group $R\bar{3}$. CsPuF₆ (Penneman, Sturgeon, Asprey & Kruse, 1965) and CsNpF₆ (Asprey, Keenan, Penneman & Sturgeon, 1966) are isostructural with CsUF₆. The present structure determination was undertaken as a means of confirming the centric nature of the structure,

and of refining this structure type on the basis of single-crystal data.

Crystals of CsUF₆ for this study were prepared by R. A. Penneman by recrystallization from cold, aqueous hydrogen fluoride solution. The crystals thus formed are pale greenish-blue rhombohedra up to 2 mm in diameter. Cleavage and twinning as reported by Sturgeon *et al.* (1965) were not observed on these crystals.

Precession photographs show the crystals to be rhombohedral with no systematic extinctions. The space group is thus $R3$, $R\bar{3}$, $R32$, $R3m$, or $R\bar{3}m$. Lattice constants were obtained from measurement of 2θ for Mo $K\alpha_1$ radiation ($\lambda = 0.70926 \text{ \AA}$) for several high order reflections with a carefully aligned single-crystal orienter on a General Electric XRD-5 spectrogoniometer. The hexagonal cell constants are $a = 8.021 \pm 0.003$, $c = 8.430 \pm 0.003 \text{ \AA}$ (the rhombohedral cell has $a = 5.417 \text{ \AA}$, $\alpha = 95^\circ 29' 5''$). These values differ significantly from those previously reported. The assumption of one formula unit per rhombohedral unit cell gives a calculated density of 5.145 g.cm^{-3} . Intensities from an entire hemisphere were measured to $2\theta \approx 50^\circ$ with Mo $K\alpha$ radiation with balanced Zr-Y filters and the fixed-counter,

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Table 1. Final least-squares parameters in CsUF₆ (rhombohedral cell)

	<i>x</i>	<i>y</i>	<i>z</i>	$\beta_{11} \times 10^4$	$\beta_{22} \times 10^4$	$\beta_{33} \times 10^4$	$\beta_{12} \times 10^4$	$\beta_{13} \times 10^4$	$\beta_{23} \times 10^4$
U	0	0	0	199 ± 3	β_{11}	β_{11}	121 ± 4	β_{12}	β_{12}
Cs	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	270 ± 4	β_{11}	β_{11}	134 ± 7	β_{12}	β_{12}
F	0.6789 ± 11	0.8036 ± 11	0.0813 ± 10	333 ± 27	364 ± 27	412 ± 29	-15 ± 42	172 ± 43	243 ± 44

$g = 3.79 \pm 0.08 \times 10^{-6}$.

fixed-crystal technique. All reflections within this range were observed and intensities of symmetry-related reflections were averaged giving a total of 187 non-equivalent reflections. The crystal, bounded by seventeen planes, had a maximum diameter of 0.027 cm, and the necessary absorption corrections were applied by the Busing & Levy (1957) method using Burnham's (1962) program modified for the present geometry.

A three-dimensional Patterson map was computed. The map indicated that the heavy atoms are in the special posi-

tions 0,0,0 and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ and that the fluorine atoms are in a set of general positions of space group $R\bar{3}$. A full-matrix least-squares refinement, including anisotropic thermal parameters, was made. The quantity minimized was $\sum w(F_o - F_c^*)^2$, where *w* is the weight based on counting statistics as given by Evans (1961), and

$$F_c^* = KF_c \left\{ 1 + g L_p \left[\frac{2(1 + \cos^2 2\theta)}{(1 + \cos^2 2\theta)^2} \right] F_c^* \right\}^\dagger,$$

where *K* = scale factor, *g* = extinction parameter according to Zachariasen (1963), *L_p* = Lorentz and polarization factor and *F_c* = the structure factor calculated in the ordinary way. The form factors for uranium and cesium were taken from Cromer & Waber (1965); that for fluorine was taken from *International Tables for X-ray Crystallography* (1962). Dispersion corrections (real part only) were applied to the uranium and cesium form factors (Cromer, 1965). The anisotropic temperature factors were in the form

$$\exp[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + hk\beta_{12} + hl\beta_{13} + kl\beta_{23})].$$

The final parameters are given in Table 1. Table 2 lists the observed and calculated structure factors for CsUF₆.

Fig. 1 is a stereo pair of the structure viewed approximately along the threefold symmetry axis. The uranium atom lies at a center of symmetry with six equidistant fluorine neighbors at 2.057 ± 0.006 Å. The fluorine atoms form an octahedral group slightly flattened along the threefold axis; the F-U-F angles are 91.9 and $88.1 \pm 0.2^\circ$. Each cesium atom has twelve fluorine neighbors: six at 3.147 ± 0.006 Å, forming a trigonal antiprism, and six at 3.101 ± 0.005 Å forming a puckered ring about the equatorial plane of the trigonal antiprism. The structure is indeed analogous to that of KOsF₆, and the centric interpretation of the absorption spectra (Reisfeld & Crosby, 1965) is confirmed.

On the basis of the paramagnetic resonance absorption of polycrystalline CsUF₆, Rigny & Plurien (1967) have

Table 2. Observed and calculated structure factors for CsUF₆

Column headings are *l*, 10*F_o*/*K* and 10*F_c**/*K* (see text).

<i>h</i>	<i>k</i>	<i>l</i>	<i>F_o</i>	<i>F_c</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i>F_o</i>	<i>F_c</i>
-4	85	77	-6 115 117	0 315 299	-4	135 135	-2 136 141	-1 409 421	
-4	85	77	-5 459 463	1 727 712	-3	515 511	-1 493 516	0 120 125	
-4	85	77	-4 218 223	2 759 740	-2	176 177	0 129 142	1 409 421	
-5	83	74	-2 154 -94	0 375 377	0	79 80	1 499 506	-5 352 355	
-4	306	306	-1 920 924	-3 217 210	1	514 510	-4 406 393	-3 333 344	
-4	306	306	-2 759 740	-2 759 740	2	176 163	-3 162 158	-2 402 423	
-4	306	306	-1 920 924	-1 325 314	0	79 80	-4 406 393	-1 131 134	
-4	306	306	0 375 377	0 766 769	-4	472 461	-3 162 158	0 414 440	
-4	306	306	0 375 377	1 181 164	-2	497 484	-2 535 451	1 126 127	
-4	306	306	0 375 377	2 698 679	-5	139 137	-1 165 164	1 126 127	
-4	306	306	0 375 377	-4 390 385	-3	160 161	0 423 423	-3 333 344	
-4	306	306	0 375 377	0 766 769	-2	497 484	1 98 105	-2 144 149	
-4	306	306	0 375 377	1 181 164	-1	132 123	2 318 317	-1 376 383	
-4	306	306	0 375 377	2 698 679	0	436 435	2 318 317	-2 130 141	
-4	306	306	0 375 377	-4 390 385	-2	497 484	-4 134 133	1 301 308	
-4	306	306	0 375 377	0 766 769	-1	132 123	-3 405 401	2 76 76	
-4	306	306	0 375 377	1 181 164	-2	497 484	-2 172 171	-1 419 432	
-4	306	306	0 375 377	2 698 679	-1	110 112	0 108 109	1 335 349	
-4	306	306	0 375 377	-4 390 385	0	436 435	2 96 104	-2 293 300	
-4	306	306	0 375 377	0 766 769	-2	497 484	-1 76 84	0 263 264	
-4	306	306	0 375 377	1 181 164	-1	132 123	1 98 106	-2 302 305	
-4	306	306	0 375 377	2 698 679	-2	497 484	1 98 106	-1 369 379	
-4	306	306	0 375 377	-4 390 385	-1	132 123	-4 122 123	-2 123 126	
-4	306	306	0 375 377	0 766 769	-2	497 484	-3 369 366	-1 369 379	
-4	306	306	0 375 377	1 181 164	-1	132 123	-2 85 86	-2 331 340	
-4	306	306	0 375 377	2 698 679	-2	497 484	0 108 109	-1 133 134	
-4	306	306	0 375 377	-4 390 385	-1	132 123	2 96 104	0 332 321	
-4	306	306	0 375 377	0 766 769	-2	497 484	-1 76 84	-2 293 300	
-4	306	306	0 375 377	1 181 164	-1	132 123	1 98 106	-2 302 305	
-4	306	306	0 375 377	2 698 679	-2	497 484	1 98 106	-1 369 379	
-4	306	306	0 375 377	-4 390 385	-1	132 123	-4 122 123	-2 123 126	
-4	306	306	0 375 377	0 766 769	-2	497 484	-3 369 366	-1 369 379	
-4	306	306	0 375 377	1 181 164	-1	132 123	-2 85 86	-2 331 340	
-4	306	306	0 375 377	2 698 679	-2	497 484	0 108 109	-1 133 134	
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-4	306	306	0 375 377	0 766 769	-2	497 484	-1 76 84	-2 293 300	
-4	306	306	0 375 377	1 181 164	-1	132 123	1 98 106	-2 302 305	
-4	306	306	0 375 377	2 698 679	-2	497 484	1 98 106	-1 369 379	
-4	306	306	0 375 377	-4 390 385	-1	132 123	-4 122 123	-2 123 126	
-4	306	306	0 375 377	0 766 769	-2	497 484	-3 369 366	-1 369 379	
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-4	306	306	0 375 377	0 766 769	-2	497 484	-3 369 366	-1 369 379	
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-4	306	306	0 375 377	0 766 769	-2	497 484	-1 76 84	-2 293 300	
-4	306	306	0 375 377	1 181 164	-1	132 123	1 98 106	-2 302 305	

Table 3. *Thermal ellipsoids in CsUF₆*

	Axis <i>i</i>	R.M.S. amplitude	<i>B_i</i>	Direction angles relative to the rhombohedral cell axes			
				α	β	γ	
Cs	1 } 2 } 3 }	0.182 ± 2 Å	2.61 ± 5 Å ²	{ 31 90 59	{ 115 138 59	{ 115 42 59	
	U	1 } 2 } 3 }	0.150 ± 1	1.79 ± 3	{ 31 90 59	{ 115 138 59	{ 115 42 59
		F	1	0.237 ± 8	4.43 ± 31	37 ± 8	124 ± 12
2	0.188 ± 9		2.79 ± 27	53 ± 8	53 ± 7	124 ± 6	
3	0.260 ± 9		5.34 ± 36	92 ± 14	55 ± 12	41 ± 10	

found that the UF₆ octahedra are axially distorted. This observation is in agreement with the present results.

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Determination of particle size and strain in cold-worked magnesium by the method of variance. By N. K.

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The method of variance was used to determine particle size and strain in cold-worked magnesium. The results are discussed and compared with those obtained by line shape analysis.

X-ray line broadening investigation of deformed metals has mainly been confined to cubic structures. Few hexagonal metals and alloys have so far been studied. Lele & Anantharaman (1964) have studied the deformation of hexagonal magnesium by the method of integral width. They did not consider the individual contributions of particle size and strain to the line broadening but attributed the entire broadening to either size effects or strain effects. Recently Mitra & Misra (1967) have determined particle size and strain in cold-worked magnesium by line shape analysis using single-line technique. No other work on X-ray line broadening study of cold-worked magnesium has been reported. In this work we present the results of the application of the method of variance to the determination of particle size and strain in deformed magnesium.

The variance of a line profile is an explicit function of the range and hence depends largely on the error in the assumed background of the profile. The dependence of variance on the background error has been discussed by Berry (1966) and by Mitra & Misra (1966). Mitra & Misra (1966) have also developed a method of correcting the back-

ground error which has been applied in the present case. The variance of a line profile corrected for background varies linearly with range (in 2θ) in a region where the intensity decreases as the inverse square of the range. Considering the entire diffraction broadening to be due to particle size and strain, the variance of a line profile in 2θ is given by Wilson (1963); this may be rearranged according to Mitra (1964):

$$\frac{W \cos \theta}{\lambda \sigma} = \frac{1}{2\pi^2 p} + \frac{n^2 \lambda}{\sigma \cos \theta} \cdot \frac{\langle e^2 \rangle}{d^2} \quad (1)$$

where $p = t/K$ is the apparent particle size, t is the real particle size, d is the interplanar distance, $d/n = \lambda/2 \sin \theta$, θ is the Bragg angle, σ is the angular range in 2θ and $\langle e^2 \rangle$ is the variance of strain. The taper parameter in equation (1) has been assumed to be zero. By proper change of axes, reflexions of the type hkl , $2h2k2l$ etc. can be treated as $00l_0$, $002l_0$ etc. reflexions for each of which the Scherrer constant $K = 1$ (Wilson, 1962). Since higher order reflexions are not available in the present case, we have used equation (1) to analyse each line separately, putting $n = 1$. The line