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Re-examination of the $\text{UZr}_6\text{FO}_{14}$ Crystal Structure

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Abstract. Orthorhombic $\text{UZr}_6\text{FO}_{14}$, isostructural with $\text{Tm}_7\text{Cl}_{15}$ and previously described with the $Pn2_1a$ space group, has been re-examined. A new description is proposed based on the same crystallographic constants [$a = 5.328$ (1), $b = 36.64$ (1), $c = 5.065$ (1) Å ($Z = 4$) and $V = 988.8$ Å³, $D_m = 6.8$ (± 0.1), $D_x = 6.91$ Mg m⁻³, $\mu(\text{Mo } K\alpha) = 26.43$ mm⁻¹] but on the centrosymmetric space group $Pnma$. $R = 0.061$ for 707 independent reflexions.

Introduction. Comparison of the results dealing with the $\text{UZr}_6\text{FO}_{14}$ structure (Papiernik, Mercurio & Frit, 1980) with those of the isostructural $\text{Tm}_7\text{Cl}_{15}$ compound (Bärnighausen, Beyer & Rinck, 1981) convinced us that the Vernier structure of $\text{UZr}_6\text{FO}_{14}$, previously described in the $Pn2_1a$ space group, could surely be better described in the centrosymmetric $Pnma$ group.

Experimental. The previously published data, i.e. 707 independent reflexions (Papiernik *et al.*, 1980), were used to refine the structure with the *SHELX* 76 program system (Sheldrick, 1976). After five cycles of calculation, for a disordered distribution of U and Zr cations over their crystallographic positions and with isotropic temperature factors for all the atoms, the residual was $R = 0.061$, the ratio of maximum least-squares shift to error being 0.009 for a mean value

0.001. As with the earlier refinement ($Pn2_1a$ group) the introduction of different degrees of cation ordering did not lead to significant improvement in the R value.

Discussion. The atomic coordinates and isotropic temperature factors are given in Table 1.† The cation–anion distances are given in Table 2. They are actually not very different from the previously published values.

† A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38381 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atom positions and isotropic temperature factors in $\text{UZr}_6\text{FO}_{14}$ (e.s.d.'s in parentheses)

Atoms						
Group	Group	x	y	z	U_{iso} (Å ²)	
$Pnma$	$Pn2_1a$					
$M(1)^*$	$M(4), M(5)$	0.3018 (3)	0.4625 (1)	0.0117 (5)	0.0041 (3)	
$M(2)$	$M(3), M(6)$	0.7307 (3)	0.3898 (1)	0.0149 (4)	0.0070 (4)	
$M(3)$	$M(2), M(7)$	0.2998 (3)	0.3191 (1)	0.0164 (5)	0.0100 (4)	
$M(4)$	$M(1)$	0.7289 (5)	$\frac{1}{2}$	0.0166 (7)	0.0101 (6)	
$X(1)$	$X(5), X(11)$	0.5779 (39)	0.4943 (5)	0.2339 (41)	0.0112 (36)	
$X(2)$	$X(6), X(12)$	0.6158 (33)	0.4378 (5)	0.8054 (33)	0.0072 (34)	
$X(3)$	$X(4), X(10)$	0.4885 (30)	0.4252 (5)	0.2818 (35)	0.0045 (32)	
$X(4)$	$X(7), X(13)$	0.3903 (32)	0.3711 (5)	0.8272 (33)	0.0061 (32)	
$X(5)$	$X(3), X(9)$	0.5294 (32)	0.3543 (5)	0.2989 (39)	0.0054 (34)	
$X(6)$	$X(8), X(14)$	0.6505 (32)	0.3085 (5)	0.8443 (33)	0.0060 (31)	
$X(7)$	$X(2), X(1)$	0.5092 (31)	0.2846 (6)	0.3028 (29)	0.0012 (28)	
$X(8)$	$X(15)$	0.3672 (53)	$\frac{1}{2}$	0.8569 (56)	0.0142 (54)	

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* $M(1)$ to $M(4) = 0.857 \text{ Zr} + 0.143 \text{ U}$.

Table 2. Main M–X and X–X distances (Å) in UZr₆FO₁₄ (e.s.d.'s in parentheses)

Symmetry operators: (i) $-\frac{1}{2} + x, y, \frac{1}{2} - z$; (ii) $\frac{1}{2} + x, y, \frac{1}{2} - z$; (iii) $1 - x, 1 - y, -z$; (iv) $x, y, -1 + z$; (v) $x, y, 1 + z$; (vi) $x, \frac{1}{2} - y, z$; (vii) $\frac{1}{2} - x, 1 - y, -\frac{1}{2} + z$.

M(1)–X(2)	2.09 (2)		
X(1 ⁱ)	2.11 (2)	X(7)–X(7 ^{vi})	2.54 (4)
X(1 ⁱⁱⁱ)	2.12 (2)	X(1)–X(1 ⁱⁱⁱ)	2.55 (4)
X(2 ^{iv})	2.17 (2)	X(3 ^v)–X(2)	2.55 (2)
X(3)	2.17 (2)	X(5)–X(7)	2.55 (3)
X(1)	2.19 (2)	X(4)–X(5 ^v)	2.58 (3)
X(3)	2.40 (2)	X(3)–X(1)	2.59 (3)
X(1 ^{iv})	2.93 (2)	X(7 ^v)–X(6)	2.59 (2)
		X(5)–X(3)	2.61 (3)
M(2)–X(4 ⁱⁱ)	2.05 (2)	X(6)–X(8)	2.62 (2)
X(2 ^{iv})	2.14 (2)	X(8 ⁱⁱ)–X(6 ^{iv})	2.64 (2)
X(3 ⁱⁱⁱ)	2.15 (2)	X(1)–X(1 ⁱ)	2.66 (3)
X(4 ^{iv})	2.16 (2)	X(4)–X(6)	2.68 (3)
X(5)	2.22 (2)	X(3)–X(3)	2.68 (2)
X(5 ⁱⁱ)	2.26 (2)	X(7)–X(8)	2.70 (3)
X(3)	2.28 (2)	X(2 ^{iv})–X(1 ⁱⁱⁱ)	2.70 (3)
X(2 ⁱⁱ)	3.15 (2)	X(5)–X(5)	2.71 (2)
		X(7)–X(7)	2.72 (2)

Table 2 (cont.)

M(3)–X(6 ⁱ)	2.03 (2)	X(2 ⁱ)–X(2 ^{iv})	2.72 (2)
X(6 ^{iv})	2.10 (2)	X(2)–X(4)	2.73 (3)
X(5 ⁱ)	2.15 (2)	X(4)–X(6 ^{iv})	2.76 (3)
X(4 ^{iv})	2.19 (2)	X(4 ^{iv})–X(4 ⁱⁱ)	2.78 (1)
X(7 ⁱ)	2.20 (2)	X(2)–X(3)	2.78 (2)
X(7)	2.22 (2)	X(1 ⁱ)–X(1 ^{iv})	2.82 (4)
X(5)	2.28 (2)	X(6 ^{iv})–X(6 ⁱ)	2.83 (1)
X(8 ^{iv})	2.68 (1)	X(8 ^{iv})–X(8 ⁱ)	2.88 (2)
		X(5)–X(6)	2.92 (3)
M(4)–X(8 ⁱⁱ)	2.03 (3)	X(2 ^{iv})–X(4 ⁱⁱ)	2.93 (3)
X(8 ^{iv})	2.09 (3)	X(1 ⁱⁱⁱ)–X(2 ⁱ)	3.00 (3)
	2×2.16 (2)		
	2×2.26 (2)		
	2×2.35 (2)		

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Single-Crystal Structure of Copper Lanthanum Telluride Cu_{0.28}LaTe₂: A Disordered Tunnel Structure

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Abstract. $M_r = 411.90$, orthorhombic, *Pbcm*, $a = 7.726$ (4), $b = 8.603$ (5), $c = 6.246$ (2) Å, $D_x = 6.59$ Mg m⁻³, $Z = 4$, $F(000) = 676$, $T = 298$ K. The structure has been refined by the least-squares method to a final R value of 0.05 for 622 independent reflections. The eightfold-coordinated La atom is inside a bicapped triangular prism of Te atoms. The polyhedra are connected so that they create pentagonal tunnels in the [001] direction which are occupied by Cu atoms in positional disorder. The Cu atoms are placed in partially occupied Cu sites, and these sites form a zigzag chain, parallel to the c axis.

Introduction. In previous investigations, Pardo & Flahaut (1971) described the ternary phase diagram Cu–La–Te, especially the quasi-binary system Cu₂Te–La₂Te₃. In order to complete the phase diagram, we are studying the system Cu–LaTe₂ (a homogeneity domain is found between LaTe₂ and SmTe₂ which exists from lanthanum to samarium). These phases are obtained by mixing Cu, La and Te elements (or Cu and LaTe₂) in appropriate proportions, and heating them in evacuated silica ampoules at 1178 K for one day, and annealing at 678 K for two days.

Experimental. Prepared from the elements using the iodine vapour transport technique at 1275 K; microprobe analysis confirmed absence of iodine and the chemical formula obtained after refinement; parallelepiped crystal (500 × 200 × 100 μm); systematic absences ($0kl$, $k = 2n + 1$; $h0l$, $l = 2n + 1$) led to the space groups *Pbcm* or *Pbc2₁*; Syntex P2₁ diffractometer, ω – 2θ scan technique, graphite-monochromated Mo $K\alpha$ radiation, $\sin \theta/\lambda$ range 0.02 to 0.7 Å⁻¹; 819 intensities collected and corrected for Lorentz, polarization and absorption effects with the crystal shape approximated by a sphere ($\mu = 25.9$ mm⁻¹); heavy-atom method. The presence of very important peaks on [001] in the Patterson function $P(u, v, w)$ shows the existence of a mirror normal to this axis. Hence the non-centrosymmetric space group *Pbc2₁* was rejected. Scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). In the first stage of the refinement, an average atom was used because the scattering factors for La and Te atoms are very close. In the second stage, they could be distinguished completely by their individual thermal factors and their surroundings.