Table 1. *Final parameters*

4 Cu	(*a*)	0	0	0
4 S	(*c*)	0·185	0·250	0·445
4 $\mathrm{O_I}$	(*c*)	0·141	0·250	0·755
4 $\mathrm{O_{II}}$	(*c*)	0·375	0·250	0·439
8 $\mathrm{O_{III}}$	(*d*)	0·129	0·069	0·307

Table 2. *Interatomic distances*

Coordination polyhedron around copper:

$\mathrm{Cu{-}O_I} = 2{\cdot}37$ Å (2×)
$\mathrm{Cu{-}O_{II}} = 2{\cdot}00$ (2×)
$\mathrm{Cu{-}O_{III}} = 1{\cdot}89$ (2×)

$\mathrm{O_{II}{-}O_{III}} = 2{\cdot}72$

$\mathrm{O_{II}{-}O'_{III}} = 2{\cdot}78$ Å
$\mathrm{O_I{-}O_{II}} = 2{\cdot}68$
$\mathrm{O_I{-}O_{III}} = 3{\cdot}13$
$\mathrm{O_I{-}O'_{III}} = 2{\cdot}93$
$\mathrm{O_I{-}O_{II}} = 3{\cdot}46$

Sulphate tetrahedron:

$\mathrm{S{-}O_I} = 1{\cdot}54$ Å
$\mathrm{S{-}O_{II}} = 1{\cdot}59$
$\mathrm{S{-}O_{III}} = 1{\cdot}46$ (2×)

$\mathrm{O_I{-}O_{III}} = 2{\cdot}48$ (2×)
$\mathrm{O_I{-}O_{II}} = 2{\cdot}49$
$\mathrm{O_{II}{-}O_{III}} = 2{\cdot}48$ (2×)
$\mathrm{O_{III}{-}O_{III}} = 2{\cdot}42$

Primes denote equivalent atoms.

The structure was refined by Fourier and difference syntheses using the intensity data published by K&R. Structure factors were calculated using the atomic scattering curves for $\mathrm{Cu^+}$ and O from the work of Berghuis *et al.* (1955) and for S from the work of Viervoll & Øgrim (1949). The curves were modified for $\mathrm{O^-}$ and $\mathrm{S^{+2}}$. The final parameters obtained are given in Table 1. Table 2 gives the interatomic distances. The values of the reliability index *R*, obtained for the zones [010] and [001] are $0{\cdot}14_3$ and $0{\cdot}16_5$ respectively, as against $0{\cdot}19_3$ and $0{\cdot}19_6$ obtained by the previous workers. Further refinement of the structure was not possible with the present intensity data. The probable error in the location of the atoms is estimated to be 0·03–0·05 Å.

From the interatomic distances given in Table 2 it is seen that $\mathrm{Cu{-}O_{II}}$ distance has decreased from 2·15 Å (K&R) to 2·00 Å; the $\mathrm{Cu{-}O_{III}}$ and $\mathrm{Cu{-}O_I}$ distances have increased from 1·87 and 2·36 Å (K&R) to 1·89 and 2·37 Å. These changes in the interatomic distances indicate with great probability that Cu has neither the (2 + 2 + 2) coordination as given by the previous authors, nor the new type of (2 + 4) coordination, but the usual (4 + 2) coordination, although the Cu–O distances in the square planar coordination are not observed to be exactly equal.

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On the unit cell of Mallinckrodt's $\mathrm{UO_3}$.

By P. M. de Wolff, *Laboratorium voor Technische Physica, Technische Hogeschool, Delft, The Netherlands*

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The X-ray powder diffraction pattern of Mallinckrodt's $\mathrm{UO_3}$ has recently been interpreted (Connolly, 1959) in terms of a monoclinic unit cell. Connolly drew attention to a number of remarkable split lines and ascribed these to pseudorhombic symmetry. However, this interpretation is weakened by an overwhelming number of multiple indexings. The total number of triplets listed is about $\frac{1}{4}$ of the number of available triplets, but this figure drops to 10% if the number of observed lines is put instead. Moreover, the first 'split line', consisting of the strong 4th and 5th line, is not even remotely accounted for by the indices stated, for which wrong calculated values are given. Only (300) with $\sin^2\theta = 0{\cdot}0314$ is acceptable here, so that one strong line remains unexplained.

A new interpretation for the same data is proposed now, based upon the quadratic form

$$10^4 \sin^2\theta = q = 124{\cdot}75(h^2+k^2) + 2{\cdot}5hk + 14{\cdot}95l^2,$$

with $h+k+l$ even. It accounts for 44 lines, which is 36% of the number of available triplets. Six lines must be ascribed to impurities. They occur at the higher angles and their intensity is from '*w*' to '*vvw*' except for $q = 1896$ and 2109. These two figure as 'medium' in Connolly's list, but they are not mentioned at all in earlier otherwise similar data (Dawson *et al.*, 1956).

Positive features of the present interpretation are:

(*a*) The split lines stand out unambiguously as hkl, $h\bar{k}l$ doublets caused by pseudosymmetry.
(*b*) The number of molecules in the body-centered unit cell

$$a = b = 6{\cdot}90,\ c = 19{\cdot}92\ \text{Å},\ \alpha = \beta = 90,\ \gamma = 90{\cdot}57^\circ,$$

corresponding to the above quadratic form, is $Z = 15$ according to the density used by Connolly, and $Z = 16{\cdot}7$ if the $\mathrm{UO_3}$ volume is taken to be equal to its value in α-$\mathrm{UO_3}$. Both figures suggest $Z = 16$. The lattice is actually face-centered orthorhombic

Table 1. *X-ray data*

I	q_o	q_c	*hkl*	*I*	q_o	q_c	*hkl*	*I*	q_o	q_c	*hkl*	*I*	q_o	q_c	*hkl*
m	139	140	101	*m*	858	858	107	*w*	1741	1742	$3\bar{2}3$	*m*	2229	2223	$3\bar{3}0$
s	238	239	004	*Bvvw*	1036	1037	206	*w*	1760	1747	1,1,10			2235	404
w	259	260	103	*w*	1224	1227	$2\bar{2}4$	*Bw*	1771	1772	323	*s*	2326	2328	332
s	307	307	$1\bar{1}2$							1778	$3\bar{1}6$	*vw*	2490	2485	$4\bar{1}5$
s	312	312	112	*w*	1255	1258	303	*w*	1788	1793	316	*m*	2529	2534	406
vs	500	499	200	*w*	1303	1300	$3\bar{1}2$	*w*	1856	1856	307	*w*	2545	2535	$4\bar{2}2$
		499	105	*w*	1310	1315	312	*m*	1896	—	—	*m*	2569	2575	422
vs	560	559	202	*w*	1337	1336	109	*w*	1914	—	—	*vw*	2740	2734	$3,\bar{1},10$
s	635	634	$2\bar{1}1$	*m*	1357	1354	$2\bar{1}7$	*w*	1947	1945	$2\bar{2}8$	*m*	2767	2761	$3\bar{3}6$
s	643	644	211					*vw*	1964	1965	228	*w*	2853	2848	329
s	758	754	$2\bar{1}3$	*Bvw*	1459	1456	208	*w*	2000	1996	400	*w*	2944	2953	408
s	761	764	213	*vw*	1491	1494	314	*vvw*	2031	—	—	*vw*	2991	—	—
m	783	785	$1\bar{1}6$	*m*	1622	1622	$3\bar{2}1$	*m*	2109	—	—	*vvw*	3076	—	—
				m	1652	1652	321	*w*	2158	2153	0,0,12	*w*	3165	3164	431

with a unit cell ($a' = 9{\cdot}70$ Å, $b' = 9{\cdot}80$ Å, $c' = c$) twice as large as the body-centered monoclinic unit cell which is used here. Since the former can accommodate 32 asymmetric units, the value $Z = 16$ for the latter involves no anomalies.

(c) In the body-centered description, the indices of all indexable lines follow the rather severe special restrictions of the space-group $I4_1/amd$. Below $q = 1800$, for instance, these restrictions account for 19 of the 31 absent indices triplets on a total of 58 available triplets in the same range. This suggests that pseudo-tetragonal symmetry applies not only to the lattice, but to the structure as well, in accordance with the equal intensities of $h\bar{k}l$ and hkl in the 'split lines'.

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Corrected values of elastic constants of sapphire.

By Walter G. Mayer and E. A. Hiedemann, *Physics Department, Michigan State University, East Lansing, Michigan, U.S.A.*

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In a recent paper Mayer & Hiedemann (1959) described various ultrasonic methods for the determination of the elastic constants of transparent single crystals. These methods were applied to ultrasonic velocity measurements in various crystallographic directions in sapphire. From the measured velocities and from the orientations supplied by the manufacturer of the samples, the six elastic constants of sapphire were calculated. More recently Wachtman *et al.* (1960) reported the values of the elastic moduli of synthetic sapphire. A comparison between their data and the results obtained by the authors showed some discrepancies which indicated that the actual orientations of some of the samples could have been different from those communicated to us by the manufacturer. A subsequent redetermination of the crystallographic orientations, performed by the National Bureau of Standards, showed this was the case for one sample.

The velocity measurements taken previously by the authors can now be interpreted on the basis of the corrected orientation of the samples. The exact Christoffel equations are used to calculate a new set of elastic constants of synthetic sapphire. The evaluating procedure given in the earlier paper is in principle incorrect and should, therefore, not be used, although it leads to practically the same values of C_{pq} in the case of sapphire. Table 1 lists the corrected values together with the average values given by Wachtman *et al.* (1960).

Table 1. *Elastic constants of synthetic sapphire*

In units of 10^{12} dyne/cm.^{2}.

C_{pq}	Wachtman *et al.*	Present work
C_{11}	4·968	4·96
C_{33}	4·981	5·02
C_{44}	1·474	1·41
C_{12}	1·636	1·35
C_{13}	1·109	1·17
C_{14}	−0·235	−0·23

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