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Tricopper(II) Tellurate(VI)

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Abstract. Cu_3TeO_6, cubic, $Ia3$, $a = 9{\cdot}537\ (1)$ Å, $Z = 8$, $\rho_x = 6{\cdot}35$ g cm^{-3}. Refinement of the structure based on 330 independent reflections gave $R = 0{\cdot}022$. The structure is built up from TeO_6 octahedra connected through Cu atoms. The Te—O lengths are 1·921 (2) Å (6×), and the Cu—O coordination distances are 1·949 (2) (2×), 2·031 (3) (2×) and 2·369 (3) Å (2×).

Introduction. The structure of Cu_3TeO_6 has been determined from powder data by Hostachy & Coing-Boyat (1968). The Te^{VI} atoms were shown to be surrounded by six chemically equivalent O atoms, as in Mg_3TeO_6 (Schulz & Bayer, 1971) and $Te(OH)_6$ (Lindqvist & Lehmann, 1973). Such simple structures are of importance for a general discussion of octahedral Te^{VI}—O coordination.

Single crystals of Cu_3TeO_6 were prepared by hydrothermal synthesis. An aqueous solution of $CuSO_4$ (1 mol dm^{-3}) and $Te(OH)_6$ (0·5 mol dm^{-3}) was held at 700°C and 900 bar for one week, whereupon suitable crystals were deposited. The crystal selected for data collection was 0·13 × 0·10 × 0·13 mm and was mounted along **c** on a two-circle Pailred diffractometer. Graphite-monochromated Mo $K\alpha$ radiation was used, and intensities were measured with the ω-scan procedure and a scan speed of 2·5° min^{-1}. The background was measured for 24 s at each end of the scan interval. The layers $hk0$–$hk12$ ($k \geq 0$) were explored out to $2\theta \simeq 60°$, giving 1543 significant reflections with $\sigma(I)/I < 0{\cdot}3$.

The data were corrected for Lorentz and polarization (program *DATAP*1; O. Lindgren, Göteborg) and absorption effects (program *DATAP*2; Coppens, Leiserowitz & Rabinovich, 1965); $\mu_{\mathrm{Mo}K\alpha} = 218{\cdot}9$ cm^{-1}.

The space group $Ia3$ was confirmed by the systematic absences. Refinement was therefore commenced with the parameters given by Hostachy & Coing-Boyat (1968). A preliminary refinement with all 1543 observed reflections gave an R of 0·035. The parameters varied were atomic coordinates, anisotropic temperature factors and an isotropic extinction factor (program *LINUS*, Coppens & Hamilton, 1970). Before the final cycles, symmetry-related reflections were averaged giving 330 independent structure factors. Since each such structure factor was in general based on six ($n = 6$) independent measurements, it was considered profitable to use true statistical $\sigma(F)$ values according to $\sigma^2(F) = \sum_{i=1}^{n} (\bar{F} - F_i)^2/n(n-1)$. A final R of 0·026 ($R_w = 0{\cdot}023$) was thus obtained and the resulting structural parameters are given in Table 1.* Scattering factors given by Cromer & Waber (1965) were used for Te^0 and by Doyle & Turner (1968) for Cu^0 and O^0. Correction for the real part of the

Table 1. *Atomic parameters*

The anisotropic temperature factor is $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$; the U_{ij} values are multiplied by 10^4.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	35 (3)	35 (3)	35 (3)	4 (3)	4 (3)	4 (3)
Cu	0·96907 (6)	0	$\frac{1}{4}$	43 (2)	54 (2)	96 (2)	0	0	38 (2)
O	0·3675 (3)	0·1742 (3)	0·3950 (3)	7 (1)	64 (9)	43 (9)	18 (8)	23 (7)	16 (6)

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33149 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

anomalous scattering was applied for Te and Cu (Cromer, 1965).

The weight analysis (Table 2) shows some variation between the different F_o intervals. The effect is, however, reasonable, since there are few observations in each interval. The final refinement was also repeated with artificial weights according to Cruickshank's (1970) formula: $\sigma^2(F) = a + F_o + cF_o^2$, with $a = 100{\cdot}0$ and $c = 0{\cdot}002$. The weight analysis did not improve, although R dropped to 0·022. It is interesting to note that some rather small, but significant, differences occurred in both positional and thermal parameters, depending on which weighting procedure was used. The most obvious example is that the z coordinate of the O atom was 0·39502 (25) and 0·39679 (19) when absolute and artificial weights, respectively, were used.

Table 2. *Agreement analysis*

N is the number of reflections in each F_o interval and $w\Delta^2 = \Sigma_N w(F_o - |F_c|)^2$, where w corresponds to (a) statistical and (b) artificial weights.

F_o interval	N	(a) $w\Delta^2$	(b) $w\Delta^2$
0·0– 25·0	58	1·82	2·80
25·0– 28·2	41	1·21	1·28
28·2– 31·7	27	1·53	0·52
31·7– 36·5	29	0·51	0·30
36·5– 41·4	26	0·75	0·42
41·4– 49·9	23	0·99	0·75
49·9– 67·6	29	0·76	0·59
67·6– 86·0	33	0·52	0·42
86·0–111·3	34	1·01	0·51
111·3–355·0	30	0·49	0·56

	(a)
$\sigma^2(F_o)$	$\Sigma_{i=1}^{n} (\bar{F}_o - F_{o,i})^2/n(n-1)$
$R = \Sigma \lVert F_o - \lvert F_c \rvert \rVert / \Sigma F_o$	0·026
$R_w = (\Sigma w \lvert F_o - \lvert F_c \rvert \rvert^2 / \Sigma w F_o^2)^{1/2}$	0·023

	(b)
$\sigma^2(F_o)$	$100{\cdot}0 + F_o + 0{\cdot}002F_o^2$
$R = \Sigma \lVert F_o - \lvert F_c \rvert \rVert / \Sigma F_o$	0·022
$R_w = (\Sigma w \lvert F_o - \lvert F_c \rvert \rvert^2 / \Sigma w F_o^2)^{1/2}$	0·031

Table 3. *Interatomic distances* (Å) *and angles* (°) *in* Cu_3TeO_6

Te–O	(6×)	1·921 (2)	O(i)–Cu–O′(ii)	166·3 (1)
Cu–O(i)	(2×)	1·949 (2)	O(i)–Cu–O(iii)	91·9 (1)
Cu–O(ii)	(2×)	2·031 (2)	O(i)–Cu–O′(iii)	120·6 (1)
Cu–O(iii)	(2×)	2·369 (3)	O(ii)–Cu–O′(ii)	95·5 (2)
O–Te–O	(6×)	94·0 (1)	O(ii)–Cu–O(iii)	75·4 (1)
O–Te–O	(6×)	86·0 (1)	O(ii)–Cu–O′(iii)	72·6 (1)
O(i)–Cu–O′(i)		96·6 (1)	O(iii)–Cu–O′(iii)	131·7 (1)
O(i)–Cu–O(ii)		85·6 (1)		

Discussion. Interatomic distances and angles are given in Table 3. The O atoms are approximately cubic close packed. The average volume per O atom is 18·1 Å³, while the value for ideal close packing is 15·6 Å³ (Pauling, 1960). This difference is due to the action of the Te and Cu coordination polyhedra.

The Cu atoms are surrounded by a distorted octahedral arrangement of O atoms (Table 3). The O atoms involved in the four strongest bonds are each shifted 0·2 Å from a planar configuration. The Cu–O interactions may thus be considered as mainly ionic, compared with the octahedral Te–O bonds, and the structure may be considered as being built up from Cu^{2+} and TeO_6^{6-} ions.

The Te atom is situated on a threefold inversion axis, *i.e.* the Te bonding orbital system has C_{3i} symmetry. The same symmetry has also been found in Mg_3TeO_6 (Schulz & Bayer, 1971), and the dimensions of the TeO_6^{6-} ion found in this structure are, within experimental error, the same as in Cu_3TeO_6. In Mg_3TeO_6 the Te–O bond is 1·913 (3) Å, and the O–Te–O angle generated by the threefold rotation is 94·2 (1)°, corresponding to 1·921 (2) Å and 94·0 (1)° in Cu_3TeO_6. It thus seems that the TeO_6 unit when occurring as a TeO_6^{6-} ion is rigid and has a definite bond distance of 1·91–1·92 Å. In $Te(OH)_6$ the mean Te–O bond distance was 1·910 (1) Å (Lindqvist & Lehmann, 1973).

The TeO_6^{6-} ion may occur in melts and in aqueous solutions under high pressure and temperatures.

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