These differences in bond distances and the deviations between the angles (*cf.* Table 7) may be a result of a higher degree of geometrical strain in the denser, three-dimensional Te_2O_5 structure. However, the differences are astonishingly small, and it is remarkable that there is no significant difference in the Te(VI)–O(3) and Te(VI)–O(6) bond distances, since O(3) and O(6) correspond to OH groups in $H_2Te_2O_6$, while they bridge two Te(VI) atoms in Te_2O_5.

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The Crystal Structure of $CuTe_2O_5$

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$CuTe_2O_5$ crystallizes in space group $P2_1/c$, with the following cell dimensions: $a=6{\cdot}871(2)$, $b=9{\cdot}322(2)$, $c=7{\cdot}602(2)$ Å, $\beta=109{\cdot}08(1)°$, and with $Z=4$. The phase problem was solved by direct methods and the final atomic parameters were obtained by full matrix least-squares refinement based on 3556 independent reflexions, an R value of 0·048 being obtained. The structure is a three-dimensional net resulting from copper and tellurium coordination polyhedra sharing oxygen atoms. Each oxygen atom interacts with three metal atoms, two of the interactions being strong and one weak. The Cu–O polyhedron may be described as a distorted octahedron with four strong bonds (Cu–O: 1·950–1·969 Å) and two weaker bonds (Cu–O: 2·305, 2·780 Å). Both independent tellurium atoms have three strong pyramidal bonds to oxygen (Te–O: 1·859–2·019 Å) and, in addition, one of them has a fourth interaction with an oxygen atom (Te–O: 2·402 Å), while the other has two weaker bonds (Te–O: 2·607, 2·733 Å).

Introduction

The structure of some double oxides of type $MO.xTeO_2$ where M = Zn or Cu have been investigated, *viz.* $ZnTeO_3$ (Hanke, 1967), $CuTeO_3$ (Lindqvist, 1972) and $Zn_2Te_3O_8$ (Hanke, 1966). The aim of this work was to determine the structure of another member of this series, $CuTe_2O_5$, which, like the above-mentioned oxides, has been prepared synthetically. Among the tellurium-containing minerals whose structures are known, denningite (Walitzi, 1965) has a chemical composition closely related to that of $CuTe_2O_5$.

X-ray investigations of $CuTe_2O_5$ were commenced by Moret, Philippot & Maurin (1969). These authors developed a method for preparing single crystals and determined the cell dimensions and space group. A single-crystal data set, consisting of 572 visually estimated intensities, was collected by Lindqvist (1971). It proved, however, difficult to solve the structure from these relatively poor film data, and more accurate and extensive diffractometer data were therefore collected and used in the investigation described in the present paper.

Experimental

The preparation of crystalline $CuTe_2O_5$ has been described previously (Moret, Philippot & Maurin, 1969). The synthesis of the crystals used in this study was performed independently, by rapid heating of a stoichiometric mixture of CuO and TeO_2 to a melt, followed by slow cooling to a temperature just below the melting point. This temperature was maintained for three hours making the formation of $CuTe_2O_5$ crystals of suitable size for single-crystal X-ray work possible.

The crystal used for the data collection was mounted along the *b* axis on an automatic Stoe four-circle diffractometer. The dimensions of the crystal are given in Table 1. The radiation used was graphite monochromated Mo $K\alpha$ radiation, and the intensities were measured using the ω–2θ scanning procedure, with a scan speed of 0·6° per min in 2θ. The background intensity was measured for 30 sec at each end of the scanning interval. A standard reflexion, 008, was measured every 50 reflexions. It appeared that there was no time dependent variation in the intensity of this standard reflexion, and only 10 of the 85 recorded values deviated more than ±2% from its mean intensity (maximum deviation: 5%). The data were collected out to $2\theta \simeq 90°$, 3900 independent reflexions being measured in all.

Table 1. *Crystal dimensions*

Boundary planes and their distances from an internal origin.

h	*k*	*l*	*d* (mm)
0	1	0	0·085
0	−1	0	0·085
1	0	0	0·020
−1	0	0	0·020
−1	0	2	0·020
1	0	−2	0·020

Crystal volume: $0·28 \times 10^{-3}$ mm³.

The measured intensity peaks were corrected for background, and assigned standard deviations $\sigma(I) = K \cdot \omega \cdot [I_{\text{peak}} + t^2 \cdot I_{\text{backgr}} + \sigma_m \cdot (I^2_{\text{peak}} + t^2 \cdot I^2_{\text{backgr}})]^{1/2}$, with $t = t_{\text{peak}}/t_{\text{backgr}}$, K = linear constant, ω = radial velocity, and with $\sigma_m = 0·025$ (assumed statistical error of each measurement). These calculations and correction for Lorentz and polarization effects were performed with a program written by Süsse (1969). Those 3556 reflexions with $\sigma(I)/I < 0·3$ were defined as observed, and the F_o values were subdivided into two groups, one more $[\sigma(I)/I < 0·1]$ and one less significant, according to $\sigma(F)_{\text{sign}} = \frac{1}{2} \cdot \sigma(I)/[\sigma(I) \cdot \text{Lp}^{-1}]^{1/2}$ and $\sigma(F)_{\text{unsign}} = \frac{1}{2} \cdot [\sigma(I) \cdot \text{Lp}^{-1}]^{1/2}$ respectively. The absorption correction, including pre-calculations for the refinement of a secondary extinction parameter, was performed with a version of the program *DATAPH* (Coppens, Leiserowitz & Rabinovich, 1965). The transmission factors, which were in the range 0·47–0·55, were not applied to the structure factors until the final stages of the refinement of the structure.

The space group reported earlier is $P2_1/c$ (Moret, Philippot & Maurin, 1969; Lindqvist, 1971), and this was checked by diffractometer measurements of reflexions $h0l$ with $l = 2n+1$ and $0k0$ with $k = 2n+1$. The cell dimensions were determined by means of a least-squares refinement based on the setting angles of seven high-angle reflexions, and were found to be identical, within the standard deviations, with those determined by Moret *et al.* (1969). Cell dimensions and other crystallographic data are given in Table 2.

Table 2. *Crystallographic data for* $CuTe_2O_5$

Unit cell	$a = 6·871\ (2)$ Å $b = 9·322\ (2)$ $c = 7·602\ (2)$ $\beta = 109·08\ (1)°$ $V = 460·1$ Å³ $Z = 4$
F.W.	398·76
Density, 20°C (Moret *et al.*, 1969)	$\varrho_o = 5·75$ g cm⁻³ $\varrho_c = 5·75$ g cm⁻³
Systematic absences	$h0l$ when $l = 2n+1$ $0k0$ when $k = 2n+1$
Space group	$P2_1/c$
Equivalent positions	$\pm(x,y,z);\ \pm(x,\frac{1}{2}-y,\frac{1}{2}+z)$.
μ(Mo $K\alpha$)	$177·3$ cm^{-3}

Structure determination and refinement

A three-dimensional Patterson summation was calculated with the program *FURIE* (Matzat, 1971). It was evident that at least the tellurium and copper atoms must occupy general positions, 4(*e*), in space group $P2_1/c$. There were, however, a number of independent ways in which the two tellurium positions could be chosen so as to give Te–Te vectors in accordance with the dominating peaks in the Patterson function. One such set of Te coordinates has been given previously (Lindqvist, 1971), but this set was subsequently found not to give a correct description of the structure. At this stage it was considered most efficient to solve the structure by means of direct methods.

After a Wilson plot (Wilson, 1942), normalized structure factors (Karle & Karle, 1966) were calculated for all reflexions with $2\theta < 60°$. $\langle|E|\rangle^2$ was standardized to 1·00, and the signs of those 223 reflexions having $|E| > 1·55$ were determined using the $\sum_2$ relationship (program *REL*, written by R. E. Long). The basic set giving the correct sign determination is shown in Table 3.

Table 3. *Statistics for the normalized structure factors and basic set used in the structure solution*

	Experimental	Theoretical	
		Cent.	Non-cent.
$\langle\lvert E\rvert\rangle$	0·821	0·798	0·886
$\langle\lvert E\rvert^2-1\rangle$	0·902	0·968	0·736
$\langle\lvert E\rvert^2\rangle$	1·000	1·000	1·000
$\lvert E\rvert > 1$	36·55%	31·73%	36·79%
$\lvert E\rvert > 2$	4·02	4·55	1·83
$\lvert E\rvert > 3$	0·00	0·27	0·01

Basic set

h k l	*E*	
0 1 4	2·54	origin fixing
−5 0 6	2·74	
5 5 3	2·63	
−1 0 6	−2·36	
1 4 3	−2·50	
4 0 0	2·80	

A Fourier summation of the 223 *E* values gave *E* maps with clearly resolved tellurium and copper positions (*R* value = 0·23). A subsequent electron density calculation using all reflexions with $2\theta < 60°$ revealed the oxygen atoms. A preliminary isotropic refinement yielded an *R* value of 0·073 which showed that the correct model had been found.

Correction was then made for absorption, and the final cycles of refinement were performed with the full-matrix least-squares program *LINUS*. This program was originally written by Busing, Martin & Levy (1962) and extended for refinement of secondary extinction parameters by Coppens & Hamilton (1970).

Table 4. *Agreement analysis after the last cycle of refinement*

The quantities $w\Delta^2$ are normalized sums, $K_{\text{norm}} \cdot (\sum w|F_o - |F_c||^2)$, and N is the number of reflexions within each F_o interval.

F_o interval	N	$w\Delta^2$
0·0–12·0	334	0·56
12·0–17·5	400	1·11
17·5–23·0	377	0·92
23·0–28·5	350	0·67
28·5–37·0	480	0·58
37·0–45·5	385	0·66
45·5–54·5	273	0·63
54·5–69·0	360	0·90
69·0–85·0	250	1·21
85·0–	347	2·91

$$R = \sum|F_o - |F_c||/\sum F_o = 0·048$$
$$R_w = (\sum w|F_o - |F_c||^2/\sum wF_o^2)^{1/2} = 0·037$$

The observations were weighted using the previously described estimates of $\sigma(F)$, with $w = 1/\sigma^2(F)$. The resulting weight analysis is given in Table 4, and the conventional *R* value converged to 0·048. (The structure was also refined after removal of 557 of the weak, less significant reflexions. The resulting parameters did not differ significantly from the previous values, and, although the *R* value dropped to 0·038, higher *e.s.d.*'s were obtained.)

The final parameter list is given in Table 5, and observed and calculated structure factors are compared in Table 6. The final value of the isosotropic extinction parameter, *g* (Coppens & Hamilton, 1970), was 0·574 (14) × 10^4.

Discussion

Atomic scattering factors due to Cromer & Waber (1965) were used for the tellurium atoms, and those given by Doyle & Turner (1968) for the copper and oxygen atoms. The tellurium and copper values were corrected for the real part of the anomalous scattering effect (Cromer, 1965).

Interatomic distances and bond angles (Tables 7 and 8) were calculated with the program *DISTAN*, written by A. Zalkin, Berkeley, California, and the drawings (Figs. 1 and 2) were obtained with the program *ORTEP* (Johnson, 1965). The calculation with these programs and with *DATAPH* and *LINUS* were performed on an IBM 360/65 computer in Göteborg, while the programs *FURIE* and *REL* were run on an Univac 1108 computer of the 'Gesellschaft für Wissenschaftliche Datenverarbeitung' in Göttingen, as was the initial refinement with a version of the Busing, Martin & Levy least-squares program (1962), modified by S. Durovic.

The $CuTe_2O_5$ structure is a rather complicated three-dimensional net of Cu–O and Te–O bonds. This is illustrated in Figs. 1 and 2, in which it can also be seen that the Cu(II) atom is strongly bonded to four oxygen atoms, while each of the two crystallographically independent Te(IV) atoms has three strong oxygen bonds. Additional weak M–O interactions (*cf.* Table 7) also occur, and each oxygen atom has two

Table 5. *Final atomic parameters in* $CuTe_2O_5$

The anisotropic temperature factor is $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$. The numbers in parentheses are the e.s.d.'s calculated by the least-squares program and refer to the least significant figures in each value.

	x	*y*	*z*
Cu	0·34117 (8)	0·48715 (5)	0·29408 (7)
Te(1)	0·13182 (4)	0·19969 (3)	0·08684 (3)
Te(2)	0·65120 (4)	0·32349 (3)	0·05685 (3)
O(1)	0·5015 (5)	0·1056 (2)	0·3232 (4)
O(2)	0·8956 (5)	0·1818 (3)	0·4649 (4)
O(3)	0·3185 (5)	0·3483 (3)	0·0931 (4)
O(4)	0·1327 (5)	0·3732 (4)	0·3560 (5)
O(5)	0·6150 (5)	0·3726 (3)	0·5067 (4)

Table 5 (*cont.*)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	0·0106 (2)	0·0063 (2)	0·0088 (2)	−0·0016 (1)	0·0052 (1)	−0·0009 (1)
Te(1)	0·00799 (8)	0·00737 (8)	0·00833 (8)	−0·00093 (6)	0·00415 (7)	−0·00073 (6)
Te(2)	0·00892 (8)	0·00670 (8)	0·00663 (8)	0·00025 (6)	0·00256 (6)	−0·00005 (6)
O(1)	0·0099 (10)	0·0106 (11)	0·0106 (11)	0·0010 (8)	0·0025 (9)	−0·0033 (9)
O(2)	0·0085 (9)	0·0155 (11)	0·0111 (11)	−0·0025 (9)	0·0053 (9)	−0·0026 (9)
O(3)	0·0113 (11)	0·0108 (11)	0·0111 (11)	−0·0044 (8)	0·0060 (9)	−0·0034 (9)
O(4)	0·0146 (12)	0·0127 (12)	0·0116 (13)	−0·0030 (9)	0·0068 (10)	0·0037 (9)
O(5)	0·0191 (13)	0·0062 (10)	0·0112 (11)	0·0014 (9)	0·0057 (10)	−0·0017 (8)

short and one long M bond. The angles around the oxygen atoms and oxygen–oxygen contacts are given in Table 8.

The covalent character of both the copper and the tellurium bonds results in an open structure. The average oxygen volume, defined as V_{cell}/(number of oxygen atoms in the cell), is approximately the same in $CuTe_2O_5$ (23·0 Å^3) as in $CuTeO_3$ (23·5 Å^3), there being distinct tunnels running through the structure of the latter (Lindqvist, 1972). However, it is useful to regard the Te(IV) lone pair, with its specific direction and its space requirements, as occupying approximately the same volume as an anion in the particular structure (Åström, 1972). In this case the average anion volume would be 16·4 and 17·6 Å^3 for $CuTe_2O_5$ and $CuTeO_3$, respectively, which is closer to the corresponding value 15·6 Å^3 in hexagonal close-packed TiO_2.

Table 6. *Observed and calculated structure factors*

The columns are h, F_o and F_c. Unobserved reflexions are marked with an asterisk.

h	F_o	F_c
H	0	0
0	0	688*
1	61	-63
2	93	-97
3	94	97
4	300	-312
5	109	-112
6	160	165
7	37	-37
8	92	95
9	89	90
10	85	-84
11	27	-28
12	4	-6*
H	1	0
1	0	-9*
2	269	-299
3	25	-27
4	83	83
5	1	2*
6	143	145
7	49	49
8	86	-86
9	17	-15
10	49	-50
11	41	-42
12	53	54
H	2	0
0	168	-180
1	101	-107
2	12	11
3	83	85
4	129	132
5	42	42
6	18	-18
7	45	-45
8	68	-69
9	23	-24
10	28	28
11	23	21
12	34	32
H	3	0
1	18	16
2	103	108
3	38	39
4	44	-43
5	17	-15
6	54	-55
7	34	-34
8	35	34
9	19	20
10	18	21
11	21	20
12	18	-20
H	4	0
0	10	12
1	35	34
2	30	-30
3	12	9
4	35	-36
5	18	-18
6	17	16
7	15	15
8	4	3*
9	21	23
10	14	-14
11	14	-11
12	5	-3
H	5	0
1	88	-92
2	112	117
3	41	-41
4	55	-56
5	76	77
6	47	-48
7	8	-15
8	56	57
9	33	-33
10	3	0*
11	28	27
12	30	-31
H	6	0
0	234	246
1	64	-65
2	76	-79
3	133	138
4	148	-155
5	34	-36
6	101	102
7	59	-59
8	25	24
9	64	65
10	66	-65
11	6	7
12	13	14
H	7	0
1	16	18
2	111	-117
3	6	-6
4	51	52
5	20	-19
6	69	69
7	23	25
8	58	-59
9	3	3*
10	25	-23
11	26	-28
H	8	0
0	113	-115
1	44	-44
2	20	19
3	21	22
4	101	104
5	29	30
6	32	-34
7	13	-13
8	55	-54
9	32	-32
10	40	40
11	2	8*
H	9	0
1	14	-11
2	141	151
3	31	31
4	65	-66
5	12	7
6	76	-79
7	48	-50
8	63	63
9	15	17
10	24	25
11	32	35
H	10	0
0	130	128
1	37	36
2	8	-12*
3	39	-40
4	87	-90
5	46	-47
6	39	40
7	26	27
8	54	53
9	30	29
10	28	-27
H	11	0
1	94	-98
2	26	-28
3	54	-54
4	20	-21
5	90	93
6	36	37
7	9	8
8	17	17
9	59	-56
10	39	-40
H	12	0
0	13	10
1	76	-77
2	20	-23
3	105	109
4	6	8
5	14	14
6	39	38
7	77	-77
8	36	-35
9	13	18
H	13	0
1	56	56
2	1	12*
3	35	34
4	14	15
5	54	-56
6	17	-15
7	8	-9
8	9	-18*
9	38	38
H	14	0
0	34	-33
1	37	39
2	8	6
3	44	-45
4	20	18
5	8	-7*
6	27	-27
7	47	47
8	3	-6*
H	15	0
1	59	-59
2	67	67
3	20	-18
4	45	-45
5	55	55
6	23	-25
7	21	-19
H	16	0
0	48	50
1	2	-3*
2	13	-11
3	14	11
4	39	-41
5	2	-6*
6	20	20
H	17	0
1	38	-34
2	15	-13
3	11	-15*
4	15	-7
5	36	36
H	18	0
0	3	-12*
1	35	-35
2	9	-2*
3	43	42
H	1	1
-13	2	-2*
-12	19	-21
-11	1	-7*
-10	7	1
-9	1	-2*
-8	41	42
-7	20	21
-6	34	-35
-5	30	29
-4	70	-69
-3	69	-66
-2	88	87
-1	4	0*
0	0	-2*
1	124	121
2	67	-70
3	67	-67
4	26	27
5	31	-29
6	2	-4*
7	70	70
8	13	-11
9	6	-11*
10	15	11
11	34	-32
12	9	-10
H	2	1
-13	30	-30
-12	36	35
-11	6	-2*
-10	19	16
-9	83	84
-8	66	-66
-7	42	-43
-6	3	1*
-5	117	-118
-4	30	28
-3	185	192
-2	12	-18
-1	125	121
0	13	17
1	202	-207
2	69	-65
3	17	15
4	58	-60
5	138	140
6	37	37
7	34	-35
8	23	22
9	50	-51
10	42	-42
11	41	39
12	4	-7*
H	3	1
-13	17	-17
-12	32	32
-11	81	80
-10	62	-62
-9	20	-18
-8	6	5
-7	150	-153
-6	72	72
-5	132	134
-4	71	-73
-3	170	174
-2	18	18
-1	302	-320
0	77	81
1	21	-19
2	109	-111
3	253	264
4	42	42
5	100	-101
6	64	64
7	106	-107
8	72	-73
9	78	78
10	1	-2*
11	20	25
12	51	53
H	4	1
-12	39	-39
-11	18	-8
-10	43	-43
-9	79	-79
-8	65	69
-7	69	70
-6	26	26
-5	134	137
-4	90	-93
-3	178	-187
-2	10	-28
-1	122	-120
0	38	40
1	252	272
2	22	20
3	38	38
4	7	-1
5	170	-175
6	37	-37
7	34	35
8	9	-14
9	86	86
10	39	37
11	40	-40
12	3	-2*
H	5	1
-12	43	-44
-11	39	-40
-10	22	25
-9	29	29
-8	62	63
-7	63	66
-6	59	-59
-5	75	-76
-4	57	-56
-3	108	-112
-2	117	118
-1	142	141
0	14	18
1	82	84
2	79	-82
3	176	-186
4	11	13
5	17	-17
6	25	29
7	120	122
8	16	13
9	34	-34
10	1	-5*
11	62	-62
12	18	-22
H	6	1
-12	25	24
-11	28	26
-10	37	36
-9	55	54
-8	36	-36
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6	126	-129
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5	2	-5*
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0	2	-11*
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2	30	-33
3	29	29
4	18	22
H	18	2
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2	17	13
H	1	3
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0	92	-91
1	103	-99
2	99	99
3	132	-135
4	16	15
5	96	94
6	43	-41
7	8	9
8	3	3*
9	65	-65
10	9	6
11	14	14
H	2	3
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-11	26	25
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-9	17	19
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-7	83	-83
-6	67	69
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-1	119	-113
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1	141	-133
2	4	9*
3	133	134
4	21	-21
5	39	41
6	23	24
7	86	-87
8	1	9*
9	1	3*
10	17	-19
11	43	42
H	3	3
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-12	13	-15
-11	19	21
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-7	26	24
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-1	74	-83
0	17	19
1	147	147
2	33	35
3	66	66
4	23	-23
5	108	-106
6	22	-29
7	24	-22
8	9	0
9	77	75
10	12	13
11	11	-2
H	4	3
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-12	76	-77
-11	43	-42
-10	29	27
-9	34	-34
-8	133	135
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-5	11	6
-4	91	-92
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-1	109	107
0	9	-1
1	232	229
2	13	-12
3	169	-171
4	23	21
5	86	-85
6	25	-23
7	122	123
8	1	6*
9	12	3
10	28	25
11	66	-63
H	5	3
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-9	71	73
-8	51	-50
-7	46	50
-6	106	-107
-5	161	-163
-4	111	111
-3	25	25
-2	27	24
-1	242	265
0	111	-123
1	127	-129
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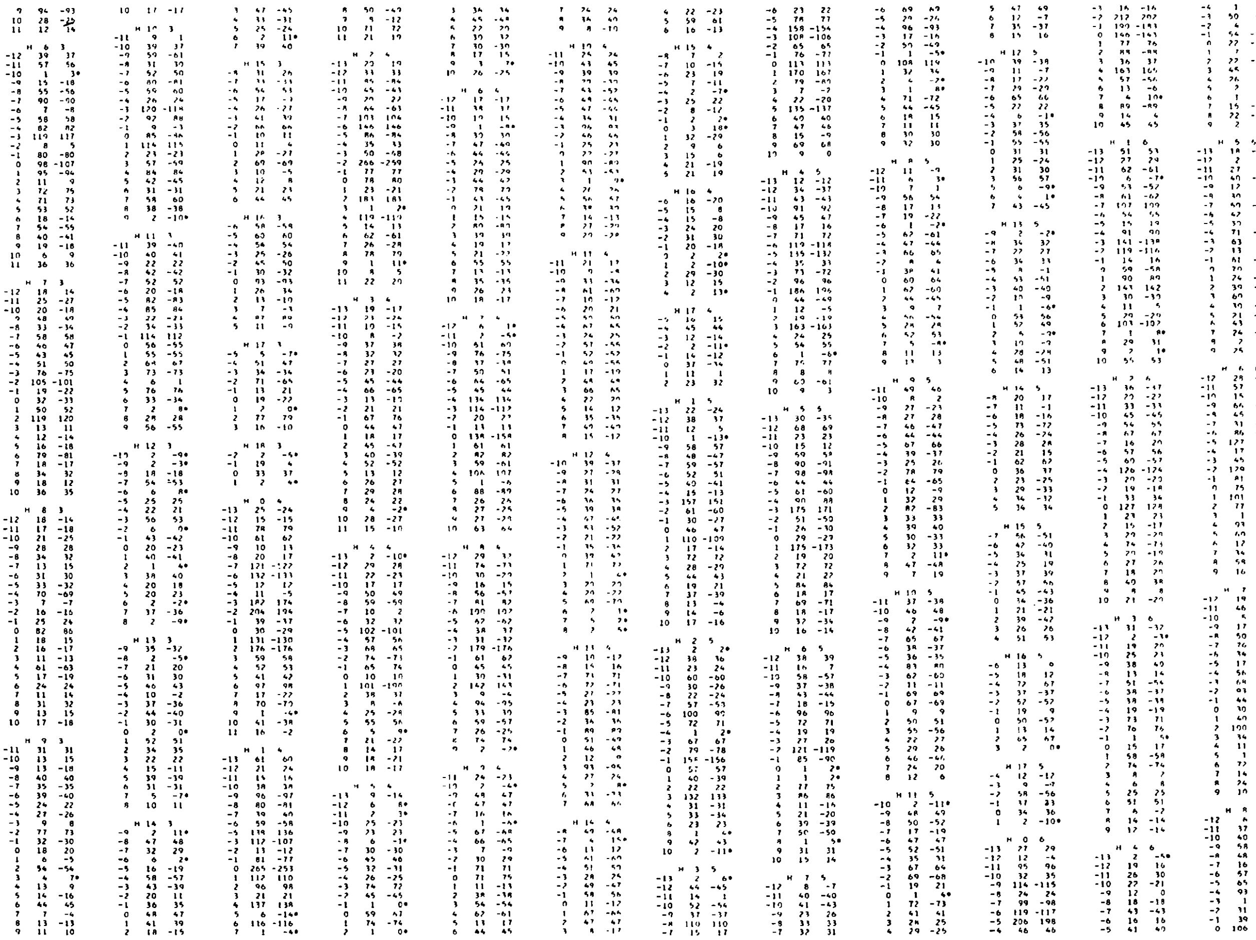
6	19	-9
7	39	41
8	17	14

Table 6 (*cont.*)



The Cu(II) atom in $CuTeO_3$ was found to have an irregular oxygen coordination (Lindqvist, 1972). In $CuTe_2O_5$ it has a more ordinary environment, with four closest oxygen atoms (Cu–O: 1·950–1·969 Å) in an approximately square-planar configuration and with two further oxygen neighbours at distances of 2·303 and 2·780 Å in directions completing a distorted octahedron. The coordination of the copper atom is in very good agreement with that found in CuO (Åsbrink & Norrby, 1970), apart from the fact that both the weak bonds in CuO are 2·780 Å. However, the Cu–O interactions in the octahedral directions can be considered very weak in comparison with the strong planar bonds, and the difference in the former interactions in the two structures can be regarded as a consequence of the geometrical arrangement in the particular structure, this having no appreciable effect on the copper–oxygen planar orbital system. In related compounds, such as $CuTeO_3.2H_2O$ (Zemann & Zemann, 1962) and $CuSeO_3.2H_2O$ (Gattow, 1958), the copper coordination is also approximately square planar, and the Cu–O distances in the octahedral directions were found to be 2·35 and 3·34 Å, and 2·27 and 3·21 Å, respectively.

Since the two independent tellurium atoms are both connected to O(2), Te_2O_5 units [*cf.* Fig. 2(*a*) and Table 7] may be regarded to be present in the structure. Such Te_2O_5 groups have also been found in denningite (Walitzi, 1965). The threefold Te coordination in these units is disturbed, since they are connected *via* copper atoms, and, moreover, since there are additional Te–O contacts of 2·402, 2·607 and 2·733 Å in the structure.

A pure threefold Te(IV) coordination may be described as a trigonal bipyramid with equal Te–O bond distances and with O–Te–O angles near 95° (Zemann, 1968), the Te(IV) lone pair being opposite to the basal plane of the pyramid. When fourfold coordination occurs, it is usually possible to describe the Te(IV) oxygen polyhedron as a distorted trigonal bipyramid, in which one of the equatorial sites is occupied by the Te(IV) lone pair. It is also possible to distinguish between the longer axial bonds and the shorter equatorial bonds, and the angle between the equatorial bonds is significantly greater than the angles

Table 6 (*cont.*)

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2	12	3
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6	20	22
7	15	7
8	50	48
H	9	6
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-10	18	11
-9	63	61
-8	26	24
-7	80	-81
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-3	103	104
-2	77	78
-1	9	-11
0	41	40
1	67	-69
2	104	-102
3	27	25
4	1	0*
5	20	27
6	78	78
7	11	-10
8	26	-23
H	10	6
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-10	15	12
-9	34	-35
-8	36	-35
-7	62	-63
-6	1	-12*
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-1	78	-77
0	58	-60
1	22	-21
2	10	-8
3	48	48
4	67	66
5	14	-3
6	9	-5
7	27	-27
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4	30	-31
5	45	-46
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1	82	83
2	42	-42
3	43	-43
5	53	-54
6	2	9*
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3	29	24
4	24	-22
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2	15	-15
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1	9	-5
2	32	33
3	16	18
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0	39	-39
3	38	39

between one axial and one equatorial bond (*cf.* review article by Zemann, 1971). Åström, Andersson, Galy & Meunier (1973) have shown that this configuration is quite natural if one considers the Te(IV) position in a hexagonal close-packed arrangement of oxygen atoms, the Te(IV) lone pair taking the place of an oxygen atom. Along these lines it was possible to calculate expected dimensions for the $Te(IV)O_4$ polyhedron, *i.e.* Te–O_{ax} = 2·22 Å, Te–O_{eq} = 1·90 Å, O_{ax}–Te–O_{ax} = 159·8° and O_{eq}–Te–O_{eq} = 99·4° (Åström *et al.*, 1973).

Zemann (1971) has pointed out that Te(IV) oxo compounds usually have three nearest neighbours with relatively constant configuration, while the distance to the fourth closest oxygen atom varies greatly (from 2·08 to 2·98 Å), but in a fairly constant direction. A simple way of deciding whether or not the fourth

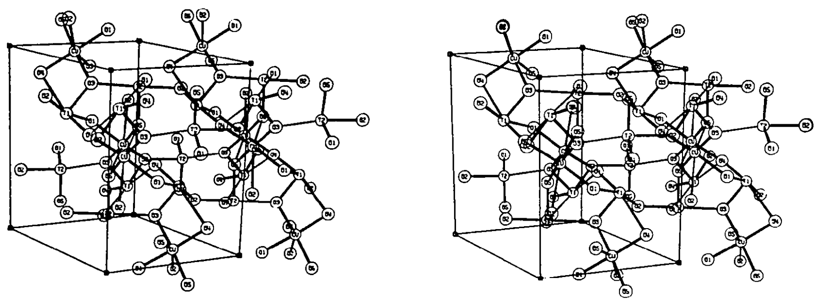

Fig. 1. Stereoscopic view of the structure.

Table 6 (*cont.*)

4	31	29
H	10	10
-9	8	-12
-8	20	19
-7	33	34
-6	50	51
-5	7	14
-4	33	-33
-3	40	-41
-2	41	-39
-1	4	-10*
0	36	35
2	24	22
3	14	1
H	11	10
-8	30	33
-7	22	22
-6	25	-24
-5	38	-37
-4	37	-38
-3	15	-12
-2	25	27
-1	40	42
0	25	25
2	32	-30
3	29	-31
H	12	10
-7	13	-10
-6	33	-35
-5	25	-25
-4	41	39
-3	17	19
-2	26	23
-1	24	28
0	39	-37
1	25	-23
2	16	-10
H	13	10
-6	46	47
-5	27	-31
-4	31	31
-3	45	45
-2	67	-68
-1	15	13
0	2	4*
H	1	11
-12	28	-29
-11	25	28
-10	33	-35
-9	5	-11*
-8	54	60
-7	22	-20
-6	7	-5
-5	48	49
-4	69	-70
-3	9	-9
-2	34	34
-1	41	-39
0	30	28
1	41	40
4	2	-3*
5	32	-30
H	2	11
-12	35	-36
-11	13	4
-10	36	36
-9	9	-6
-8	37	36
-7	13	8
-6	65	-64
-5	11	8
-4	4	-9*
-3	35	-31
-2	77	76
-1	6	7
0	25	-24
1	32	31
4	37	37
5	8	-12
H	3	11
-11	13	12
-10	44	45
-9	12	-14
-8	60	-60
-7	7	-11
-6	40	-36
-5	1	-4*
-4	90	90
-3	13	12
-2	16	12
-1	16	17
0	80	-81
5	33	33
H	4	11
-11	2	-6*
-10	59	-61
-9	1	1*
-8	52	-54
-7	21	-18
-6	103	102
-5	12	6
-4	8	12
-3	38	38
-2	101	-102
-1	39	-36
0	33	35
4	43	-43
5	2	2*
H	5	11
-11	2	-3*
-10	57	-59
-9	9	-6
-8	99	101
-7	1	6*
-6	35	33
-5	29	28
-4	109	-110
-3	49	-48
-2	23	22
-1	35	-35
0	79	79
3	2	2*
4	24	-26
H	6	11
-11	2	6*
-10	30	33
-9	38	38
-8	40	41
-7	10	-10
-6	52	-51
-5	40	-40
-4	32	-32
-3	8	15
-2	58	56
-1	38	39
0	17	12
3	28	30
4	6	4*
H	7	11
-10	11	14
-9	19	-16
-8	2	-7*
-7	57	-58
-6	29	-35
-5	40	41
-4	18	17
-3	36	36
-2	41	42
-1	37	-39
0	38	-37
2	23	-24
3	21	20
4	34	37
H	8	11
-10	20	-19
-9	29	-32
-8	6	-5
-7	15	2
-6	14	14
-5	46	47
-4	16	4
-3	17	-17
-2	1	-6*
-1	39	-39
0	14	-16
2	2	4*
3	23	18
H	9	11
-9	2	-3*
-8	12	-12
-7	36	38
-6	11	-10
-5	17	-9
-4	17	17
-3	27	-28
-2	9	-11
-1	29	32
0	22	-20
1	18	14
2	25	20
3	26	-28
H	10	11
-8	25	-26
-7	24	-27
-6	53	54
-5	29	-33
-4	18	-14
-3	51	51
-2	46	-45
-1	2	-1*
0	44	44
1	41	-41
2	17	12
H	11	11
-7	24	-23
-6	14	13
-5	31	31
-4	64	-65
-3	11	1
-2	21	20
-1	36	-37
0	36	37
1	24	30
H	12	11
-6	32	-30
-5	2	-6*
-4	18	-15
-3	5	-3*
-2	37	39
-1	2	6*
H	0	12
-11	71	-73
-10	32	34
-9	23	23
-8	12	9
-7	85	84
-6	16	-17
-5	79	-81
-4	14	14
-3	61	-63
-2	8	-12
-1	98	100
0	14	9
3	76	-76
4	26	-28
H	1	12
-11	31	32
-10	14	16
-9	65	67
-8	13	-5
-7	69	-70
-6	5	-12*
-5	56	-57
-4	13	-11
-3	88	87
-2	24	23
-1	19	16
0	28	28
1	75	-76
2	37	-33
3	12	13
4	23	-20
H	2	12
-11	54	54
-10	11	10
-9	52	-54
-8	1	-2*
-7	39	-38
-6	28	-29
-5	70	71
-4	25	24
-3	9	3
-2	33	32
-1	55	-57
0	43	-42
1	14	13
2	12	-10
3	30	28
4	45	41
H	3	12
-11	14	-11
-10	22	-20
-9	32	-34
-8	11	3
-7	22	22
-6	16	21
-5	27	31
-4	1	4*
-3	37	-38
-2	17	-15
-1	23	-23
0	1	-3*
1	28	31
2	23	19
3	2	6*
4	4	4*
H	4	12
-10	6	-2
-9	16	-14
-8	35	32
-7	16	17
-6	20	-21
-5	12	15
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-3	32	-33
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-1	7	8
0	11	-6
1	32	33
2	13	-9
3	15	-17
H	5	12
-10	9	13
-9	26	-24
-8	15	16
-7	10	16
-6	27	-26
-5	27	24
-4	1	-1*
-3	31	-32
-2	22	26
-1	9	-3
0	20	-22
1	36	33
2	2	-10*
3	25	-18
H	6	12
-10	21	24
-9	2	7*
-8	25	-25
-7	58	57
-6	14	-14
-5	44	-43
-4	38	38
-3	29	-30
-2	22	-22
-1	66	64
0	22	-23
1	2	-8*
2	35	34
3	42	-44
H	7	12
-9	51	54
-8	2	6*
-7	59	-59
-6	15	11
-5	29	-30
-4	35	-34
-3	74	75
-2	8	2
-1	2	2*
0	34	36
1	50	-51
2	24	-25
H	8	12
-9	44	-46
-8	14	8
-7	41	-42
-6	25	-27
-5	65	66
-4	7	6
-3	16	10
-2	33	35
-1	64	-61
0	24	-24
1	4	11*
2	20	-20
H	9	12
-8	6	10
-7	37	36
-6	11	15
-5	49	51
-4	10	1
-3	57	-58
-2	9	-13
-1	31	-27
0	2	-12*
1	55	55
H	10	12
-7	33	34
-6	2	-10*
-5	23	-26
-4	26	-28
-3	37	-39
-2	15	14
-1	35	37
0	21	20
H	11	12
-5	6	-5
-4	2	0*
-3	15	14
-2	55	57
H	1	13
-10	17	20
-9	2	2*
-8	20	20
-7	18	14
-6	23	-26
-5	11	-10
-4	11	-11
-3	14	-15
-2	21	22
-1	19	14
0	2	6*
1	2	6*
2	13	-12
H	2	13
-10	53	55
-9	11	-9
-8	25	-26
-7	10	12
-6	59	-62
-5	6	2*
-4	49	47
-3	12	-10
-2	37	36
-1	21	19
0	60	-60
1	2	5*
2	21	-11
H	3	13
-10	11	6
-9	2	-3*
-8	94	-98
-7	28	29
-6	42	42
-5	24	-26
-4	91	92
-3	10	11
-2	84	-80
-1	24	24
0	35	-38
1	41	-42
2	75	75
H	4	13
-9	2	4*
-8	29	28
-7	10	4
-6	63	63
-5	12	11
-4	58	-59
-3	13	-2
-2	42	-41
-1	22	-19
0	62	62
1	16	15
2	2	8*
H	5	13
-9	25	21
-8	49	51
-7	2	17*
-6	40	-42
-5	24	-26
-4	37	-41
-3	14	-19
-2	43	45
-1	29	31
0	22	21
1	19	17
H	6	13
-9	9	-8
-8	2	-8*
-7	23	-21
-6	53	-52
-5	6	0
-4	34	37
-3	9	11
-2	39	39
-1	12	9
0	42	-43
1	15	-13
H	7	13
-8	33	-34
-7	6	2
-6	13	12
-5	30	27
-4	32	35
-3	2	-2*
-2	23	-22
-1	22	-22
0	27	-23
H	8	13
-7	40	43
-6	2	-5*
-5	17	11
-4	4	7*
-3	56	-54
-2	2	1*
-1	14	6
H	9	13
-6	11	7
-5	52	-55
-4	25	28
-3	7	2
-2	33	-31
H	0	14
-9	83	87
-8	27	-27
-7	2	-2*
-6	8	*
-5	96	-96
-4	2	-1*
-3	56	59
-2	27	-25
-1	67	66
0	29	29
H	1	14
-9	2	6*
-8	18	-17
-7	74	-78
-6	3	-1*
-5	24	23
-4	7	4
-3	67	67
-2	12	17
-1	40	-44
0	12	-7
H	2	14
-8	10	-11
-7	8	4
-6	28	27
-5	41	40
-4	2	0*
-3	14	-12
-2	17	-20
-1	40	-33
0	2	2*
H	3	14
-9	7	2*
-8	17	15
-7	32	34
-6	2	7*
-5	15	-14
-4	11	-9
-3	33	-33
-2	13	-5
-1	25	21
0	2	0*
H	4	14
-8	2	1*
-7	18	-16
-6	2	2*
-5	19	-19
-4	19	-5
-3	10	14
-2	2	0*
-1	2	2*
H	5	14
-7	33	35
-6	21	-15
-5	12	-11
-4	33	32
-3	26	-26
-2	2	-7*
-1	21	25
H	6	14
-6	34	32
-5	57	-60
-4	4	16*
-3	36	37
-2	36	-39
H	7	14
-5	10	15
-4	2	-7*
H	1	15
-6	13	-15
-5	8	12
-4	17	-17
-3	2	6*
H	2	15
-5	12	-10
-4	54	55

oxygen neighbour has a significant influence on the Te(IV) bonding orbitals, and thus a way of qualitatively estimating the strength of the fourth Te–O interaction, would be to observe the strong Te–O bond on the opposite side of the tellurium atom and the angle between the two other short Te–O bonds. If this bond is longer than the other two and if the angle is significantly larger than the other two angles in the Te pyramid, elements of fourfold coordination can be regarded as being present.

In CuTe$_2$O$_5$ the fourth oxygen neighbour of Te(2) is O′(3) at a distance of 2·402 Å. From Table 7 it is evident that Te(2) shows fourfold geometry, thus indicating that the Te(2)–O′(3) interaction is of considerable strength. The M–O(3)–M angles (Table 8) are all close to 120° which is to be expected for an oxygen atom with bonds to three metal atoms. Similar conditions hold for the coordination of Te in denningite (Walitzi, 1965) and of Te(2) in CuTeO$_3$ (Lindqvist, 1972), where the fourth Te–O bond distances are 2·36 Å and 2·32 Å respectively.

The oxygen arrangement around Te (1) in CuTe$_2$O$_5$ is closer to pure threefold coordination, as a consequence of the longer distances to the additional oxygen atoms O′(1) (2·733 Å) and O′(4) (2·607 Å). Such distances have, however, been reported to correspond to significant interatomic interactions, for example in Te(C$_6$H$_4$O$_2$)$_2$ (Lindqvist, 1967) and in Te$_2$O$_5$ (Lind-

Table 7. *Tellurium and copper coordination distances* (Å) *and angles* (°)

The standard deviations are 0·003 Å for all distances and lie in the range 0·09–0·14° for all angles. The notation is in accordance with Fig. 2.

Te(1)–O(3)	1·877	Cu–O(5)	1·950
Te(1)–O(4)	1·883	Cu–O(1)	1·952
Te(1)–O(2)	1·931	Cu–O(4)	1·961
Te(1)–O′(4)	2·607	Cu–O(3)	1·969
Te(1)–O′(1)	2·733	Cu–O′(5)	2·305
		Cu–O(2)	2·780
Te(2)–O(1)	1·859		
Te(2)–O(5)	1·866	O(1)–Cu–O(2)	65·8
Te(2)–O(2)	2·019	O(1)–Cu–O(3)	86·2
Te(2)–O′(3)	2·402	O(1)–Cu–O(4)	166·7
		O(1)–Cu–O(5)	90·4
O′(1)–Te(1)–O(2)	162·6	O(1)–Cu–O′(5)	97·8
O′(1)–Te(1)–O(3)	74·9	O(2)–Cu–O(3)	90·0
O′(1)–Te(1)–O(4)	102·2	O(2)–Cu–O(4)	102·7
O′(1)–Te(1)–O′(4)	85·4	O(2)–Cu–O(5)	91·0
O(2)–Te(1)–O(3)	92·8	O(2)–Cu–O′(5)	162·7
O(2)–Te(1)–O(4)	91·0	O(3)–Cu–O(4)	87·2
O(2)–Te(1)–O′(4)	79·0	O(3)–Cu–O(5)	175·7
O(3)–Te(1)–O(4)	94·6	O(3)–Cu–O′(5)	94·5
O(3)–Te(1)–O′(4)	72·3	O(4)–Cu–O(5)	96·7
O(4)–Te(1)–O′(4)	162.8	O(4)–Cu–O′(5)	94·2
		O(5)–Cu–O′(5)	83·3
O(1)–Te(2)–O(2)	86·6		
O(1)–Te(2)–O′(3)	80·0		
O(1)–Te(2)–O(5)	99·0		
O(2)–Te(2)–O′(3)	166·6		
O(2)–Te(2)–O(5)	88·6		
O′(3)–Te(2)–O(5)	92·8		

Table 8. *Oxygen contacts below* 3·6 Å *and* M–O–M *angles*

The last column in the distance list represents the metal atoms to which the two oxygen atoms are bonded. Strong and weak bonds are indicated as = and –, respectively. The standard deviations of the angles lie in the range 0·10–0·18°.

O(1)–O(2)	2·662 (4) Å	=Te(2)=, =Cu–
O(1)–O(3)	2·678 (4)	=Cu=
O(3)–O(4)	2·710 (4)	=Cu=, =Te(1)–
O(2)–O(5)	2·715 (4)	=Te(2)=
O(2)–O(4)	2·719 (5)	=Te(1)=
O(2)–O(3)	2·760 (4)	=Te(1)=
O(3)–O(4)	2·762 (4)	=Te(1)=
O(1)–O(5)	2·768 (5)	=Cu=
O(1)–O(3)	2·770 (4)	=Te(2)–
O(1)–O(5)	2·834 (4)	=Te(2)=
O(5)–O(5)	2·839 (6)	=Cu–
O(1)–O(3)	2·855 (4)	=Te(1)–
O(4)–O(5)	2·922 (5)	=Cu=
O(2)–O(4)	2·931 (5)	=Te(1)–
O(3)–O(5)	3·114 (4)	=Te(2)–
O(4)–O(5)	3·132 (5)	=Cu–
O(3)–O(5)	3·146 (5)	=Cu–
O(1)–O(5)	3·214 (4)	=Cu–
O(1)–O(1)	3·339 (6)	
O(2)–O(3)	3·407 (4)	=Cu–
O(2)–O(5)	3·424 (5)	=Cu–

Table 8 (*cont.*)

Cu══O(1)=Te(2)	115·0°
Cu══O(1)-Te(1)	114·6
Te(1)-O(1)=Te(2)	128·2
Te(1)=O(2)=Te(2)	120·8
Cu——O(2)=Te(1)	156·8
Cu——O(2)=Te(2)	82·4
Cu══O(3)=Te(1)	112·7
Cu══O(3)-Te(2)	108·4
Te(1)=O(3)-Te(2)	126·4
Cu══O(4)=Te(1)	130·1
Cu══O(4)-Te(1)	87·8
Te(1)=O(4)-Te(1)	120·5
Cu══O(5)=Te(2)	121·4
Cu══O(5)-Cu	96·7
Cu——O(5)=Te(2)	128·4

qvist & Moret, 1973). The above criteria for four-coordination holds rather well for O′(1), and better for O′(1) than for the slightly closer O′(4). The M–O(1)–M angles are also consistent with a Te(1)–O′(1) interaction. These arguments thus suggest that the Te(1)–O′(1) force is stronger than that between Te(1) and O′(4). This might be feasible, bearing in mind that geometrical strains imposed by the stronger M–O bonds certainly influences these distances of 2·6–2·8 Å more than the corresponding weak Te–O interactions.

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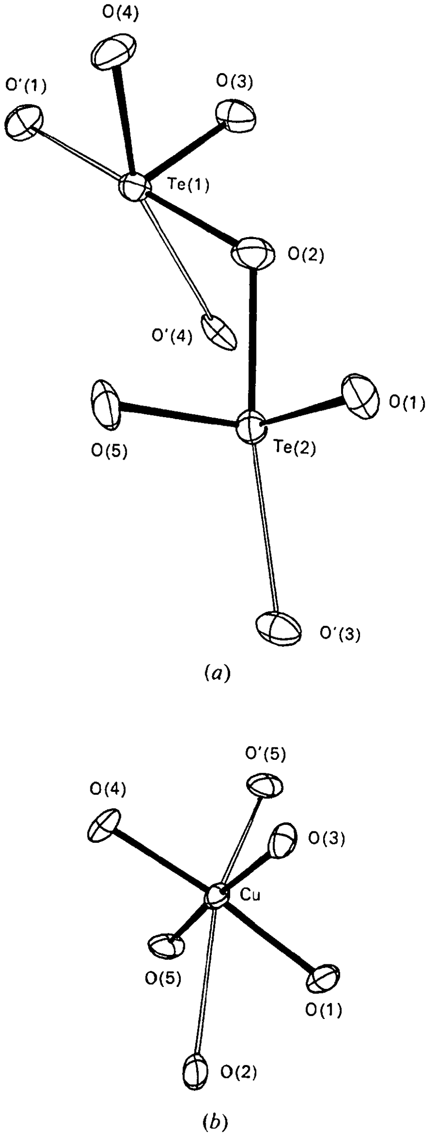

Fig. 2. Coordination of (*a*) the two tellurium and (*b*) the copper atoms.

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