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The Crystal Structure of $CuTeO_3$

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$CuTeO_3$ crystallizes in space group *Pmcn* with the cell dimensions $a = 7.604$, $b = 5.837$, and $c = 12.705$ Å and with $Z = 8$. Its structure has been determined by means of three-dimensional Patterson and electron density summations, a final R value of 0.084 being obtained after full matrix least squares refinement.

The copper and tellurium atoms are linked together by oxygen atoms to form a three-dimensional network. There are two chemically different tellurium atoms in the structure, both of which are strongly bonded to three oxygen atoms at Te – O distances of 1.86 – 1.96 Å, while one of them has in addition a fourth oxygen neighbour, at a longer Te – O distance of 2.32 Å. The copper atom does not exhibit a regular coordination and is surrounded by four nearly equi-distant oxygen atoms (Cu – O distances of 1.94 – 1.98 Å) and a fifth at 2.38 Å.

In a recent investigation of the $CuO - TeO_2$ system, Moret, Philippot and Maurin [1] succeeded in preparing single crystals of two new phases with the compositions $TeO_2 \cdot CuO$ and $2TeO_2 \cdot CuO$, for which they also determined cell dimensions and possible space groups. The present study deals with the crystal structure determination of the first of these two phases, $CuTeO_3$. Crystals of both phases, suitable for single crystal X-ray work, have kindly been provided by Dr. Philippot, and a corresponding investigation of $CuTe_2O_5$ is in progress.[2]

Compounds similar to $CuTeO_3$ have been studied by Hanke,[3] who determined the structure of $ZnTeO_3$, and by Zemann and Zemann,[4] who showed that the mineral teinite had the formula $CuTeO_3.2H_2O$ and a structure isomorphous with that of chalcomenite, $CuSeO_3.2H_2O$.[5] It therefore seemed interesting to determine in which respects the structure of the anhydrous $CuTeO_3$ phase differed from that of teinite, and also to investigate those structural differences which might arise from the presence of the zinc and copper ions in $ZnTeO_3$ and $CuTeO_3$, respectively.

EXPERIMENTAL

A single crystal with the dimensions given in Table 1 was mounted along the c axis, and intensities corresponding to $hk0-hk11$ were registered using Weissenberg multiple film techniques and Cu$K\alpha$ radiation.

Table 1. Crystal dimensions. d is the distance to each face from an arbitrary origin inside the crystal.

Boundary face	d (mm)
0 0 1	0.062
0 0 −1	0.062
1 0 0	0.050
1 1 0	0.040
1 1 −1	0.045
1 1 1	0.045
−1 2 2	0.040
−1 2 −2	0.040
−1 0 0	0.050
−1 −1 0	0.045
0 −1 −2	0.035
0 −1 1	0.045
1 −1 0	0.048

Crystal volume: 6.0×10^{-4} mm^3

A total of 546 independent reflections were estimated visually by comparison with an intensity strip, prepared by timed exposures of a suitable reflection from the crystal. The differently exposed films for each layer line were brought on to a common scale by means of a least squares scaling procedure,[6] using the weighting function

$$w=\begin{cases}(kI_j)^{-1/2}, I_j<k\\ k^{1/2}I_j^{-3/2}, I_j\geq k\end{cases}$$

where I_j is the intensity on the j:th film and k was assigned a value within that part of the intensity strip where the most sensitive estimations could be made. The scale factors

Table 2. Crystallographic data for $CuTeO_3$.

Unit cell:[1]	a = 7.604(6) Å
	b = 5.837(4) Å
	c = 12.705(6) Å
	U = 564 Å^3
	Z = 8
Formula weight:	M = 239.14
Density (20°C):[1]	D_m = 5.62 g cm^{-3}
	D_x = 5.637 g cm^{-3}
Systematic absences:	$h0l$ when $l=2n+1$
	$hk0$ when $h+k=2n+1$
Space group:	$Pmcn$
Equivalent positions:	8(d) $\pm(x,y,z)$; $\pm(\frac{1}{2}+x,\frac{1}{2}+y,\frac{1}{2}-z)$;
	$\pm(\frac{1}{2}+x,-y,-z)$; $\pm(x,\frac{1}{2}-y,\frac{1}{2}+z)$;
	4(c) $\pm(\frac{1}{4},y,z)$; $\pm(\frac{1}{4},\frac{1}{2}-y,\frac{1}{2}+z)$;
	4(b) $(0,0,\frac{1}{2})$; $(\frac{1}{2},\frac{1}{2},0)$; $(\frac{1}{2},0,\frac{1}{2})$; $(0,\frac{1}{2},0)$;
	4(a) $(0,0,0)$; $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; $(\frac{1}{2},0,0)$; $(0,\frac{1}{2},\frac{1}{2})$;
Linear absorption coefficient:[7]	μ = 940 cm^{-1} (Cu$K\alpha$ radiation)

between the layer lines were initially assigned values in accordance with the exposure times.

Crystallographic data for $CuTeO_3$ are given in Table 2.

STRUCTURE DETERMINATION AND REFINEMENT

From a three-dimensional Patterson calculation, the eight tellurium atoms in the unit cell were found to occupy two positions 4(*c*) in space group *Pmcn* (*cf.* Table 2). The coordinates of the copper and oxygen atoms were then deduced from successive electron density calculations, in agreement with the centric space group. The acentric space group, $P2_1cn$, was not therefore considered any further.

A preliminary isotropic refinement of the structure, including scale factors for the 12 layer lines, ($R = \sum||F_o| - |F_c||/\sum|F_o| = 0.145$) showed clearly that the data suffered from considerable errors due to absorption and possibly also to extinction. An absorption correction was applied using the Gaussian integration method, the crystal being divided into $4 \times 6 \times 4$ grid points (*cf.* Table 1). This coarse division was considered sufficient in view of the precision level of the visually estimated film data. The resulting transmission factors varied between 0.010 and 0.10. When the isotropic refinement was repeated with data corrected for absorption, the results improved ($R = 0.128$), but there were still large errors due to extinction. To correct for these, Zachariasen's formula [8,9] for isotropic secondary extinction, as applied by Åsbrink and Werner,[10] was used. The C coefficient required in this formula was chosen after comparison of the results of several refinements using different C values close to a preliminary value estimated from the errors in a number of the strongest reflections. The best agreement was obtained for $C = 1.4 \times 10^{-3}$, giving an R value of 0.108.

Table 3. Final atomic parameters. The anisotropic temperature factor is

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + hka^*b^*U_{12} + hla^*c^*U_{13} + klb^*c^*U_{23})\}.$$

Standard deviations, referring to the least significant figures, are given in parentheses.

Atom	x/a	y/b	z/c
Te_1	1/4	0.1702(3)	0.1141(2)
Te_2	3/4	0.1040(3)	0.1630(2)
Cu	0.5454(4)	0.1607(5)	0.4105(3)
O_1	0.430(2)	0.338(2)	0.046(1)
O_2	0.447(3)	0.411(3)	0.325(2)
O_3	3/4	0.110(3)	0.317(2)
O_4	3/4	0.428(3)	0.481(2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te_1	0.007(1)	0.015(1)	0.013(2)	0	0	0.000(1)
Te_2	0.006(1)	0.015(1)	0.011(2)	0	0	0.000(1)
Cu	0.018(2)	0.020(2)	0.011(2)	0.008(2)	0.008(2)	0.004(2)
O_1	0.014(6)	0.018(7)	0.034(11)	−0.007(11)	0.003(13)	0.008(13)
O_2	0.037(10)	0.041(10)	0.023(12)	0.051(17)	0.027(16)	0.049(16)
O_3	0.007(10)	0.021(10)	0.007(14)	0	0	−0.019(16)
O_4	0.022(10)	0.017(9)	0.002(13)	0	0	−0.039(15)

Table 4. Observed and calculated structure factors. The columns are k, $|F_o|$, and F_c, respectively. * indicates reflections excluded from the refinement.

0 K 0
2 112 -103
4 192 -255*
6 73 75

1 K 0
3 166 160
5 53 54
7 125 -115

2 K 0
0 157 -183
2 29 -26
4 95 86
6 38 35

3 K 0
1 53 69
3 161 -161
5 108 -100
7 165 136*

4 K 0
0 441 382*
2 38 -36
4 165 -158
6 31 26

5 K 0
1 49 46
3 116 116
5 15 9

6 K 0
0 304 -287
2 39 37
4 129 130

7 K 0
1 73 68
3 90 -96
5 97 -85

8 K 0
0 124 135
4 67 -72

9 K 0
1 17 14

0 K 1
1 76 68
2 277 -280
3 34 22
4 65 69
5 42 -42
6 46 50
7 29 -26

1 K 1
1 96 115
2 42 -38
4 143 127
5 115 -122
6 33 -30
7 21 -16

2 K 1
1 153 -214*
2 143 193*
3 199 228
4 28 26
5 20 -16
6 37 37
7 36 -33

3 K 1
2 48 -48
3 90 -91
4 81 -79
5 127 118
6 38 34
7 32 30

4 K 1
1 94 98
2 186 -213
3 68 -71
4 32 32
5 16 -12
6 45 47

5 K 1
1 106 103
2 78 -79
3 27 -21
4 128 124
5 113 -97
6 21 -20

6 K 1
1 88 -79
2 140 147
3 68 67
4 23 -14
5 20 17

7 K 1
1 20 -17
2 45 -39
3 54 -51
4 56 -51
5 88 89

8 K 1
1 88 90
2 107 -114
3 104 -106

9 K 1
1 42 41
2 35 -32

0 K 2
1 99 -99
2 84 -77
3 52 -53
5 31 31
6 68 70
7 18 15

1 K 2
0 46 -95*
1 52 -61
2 111 140*
3 46 -45
4 21 -17
5 21 20
6 121 -138
7 27 23

2 K 2
0 104 118
1 234 332*
2 26 -20
3 104 113
4 69 -65
5 123 -128
7 25 22

3 K 2
0 63 -67
1 78 88*
2 45 -45
3 58 57
4 65 66
5 36 -32
6 66 67
7 20 -19

4 K 2
0 34 -27
1 128 -140
2 29 -27
3 63 -63
4 36 28
5 60 54
6 40 36

5 K 2
0 120 -119
1 19 -18
2 118 133
3 31 -30
4 18 10
6 151 -145

6 K 2
0 23 18
1 146 144
2 26 26
3 61 66
4 27 -28
5 71 -63

7 K 2
0 39 -38
1 66 64
2 41 -41
3 44 42
4 53 49
5 32 -27

8 K 2
0 60 -52
1 137 -145
3 59 -58
4 34 33

9 K 2
0 38 -29
1 21 -19
2 57 62

0 K 3
1 199 -190
2 226 -229
3 117 126
4 117 151*
5 56 57

1 K 3
1 33 -40
2 19 -18
3 64 62
4 98 -98
5 38 -38
6 51 53
7 11 -8

2 K 3
1 98 107
2 17 4
3 102 -114
4 35 -29
5 41 -41
6 17 16
7 14 12

3 K 3
1 118 129
2 81 89
3 196 -192
4 89 84
5 71 69
6 60 -57

4 K 3
1 109 -118
2 121 -134
3 91 87
4 100 96
5 51 45

5 K 3
1 21 13
2 15 -6
3 20 -7
4 84 -83
5 23 -18
6 44 45

6 K 3
1 127 110
2 82 74
3 93 -96
4 70 -64
5 50 -41

7 K 3
1 72 71
2 51 48
3 116 -118
4 69 68
5 41 46

8 K 3
1 70 -74
2 31 -35
3 60 61
4 27 33

9 K 3
1 20 -18
2 29 -30

0 K 4
1 108 87
2 105 88
3 80 76
4 112 131
5 33 -28
6 65 -70
7 36 -37

1 K 4
0 255 -241
1 53 58
3 69 -65
4 97 100
5 44 -43
6 12 7
7 78 80

2 K 4
0 140 139
1 19 22
2 40 -38
3 98 -97
4 84 -82
5 61 -55
6 26 20
7 72 72

3 K 4
0 27 6
1 123 -137
2 46 49
3 62 60
4 31 -26
5 82 89
6 55 -53

4 K 4
0 245 -234
1 62 60
2 60 58
3 69 82
4 98 98
5 15 -10
6 51 -50

5 K 4
0 247 -237
2 25 23
3 52 -55
4 101 106
5 18 -13
6 17 -13

6 K 4
0 160 157
1 22 -17
2 44 -40
3 62 -59
4 76 -69
5 15 -17

7 K 4
0 48 44
1 79 -79
2 23 22
3 44 43
4 35 -33

8 K 4
0 101 -109
2 28 24
3 61 60

9 K 4
0 87 -90
1 26 25

0 K 5
1 108 84
2 157 159
3 20 -14
5 61 -67
6 45 -41

1 K 5
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2 141 182*
3 34 -31
4 82 -81
5 101 113
7 24 25

2 K 5
1 91 91
2 158 -207*
3 155 -179
4 20 -15
5 90 87
6 44 40

3 K 5
1 104 104
2 77 -76
3 37 -36
5 84 -83

4 K 5
1 22 15
2 119 137
3 53 49
4 21 17
5 72 -66
6 41 -36

5 K 5
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2 166 184
3 48 -44
4 100 -100
5 111 102

6 K 5
2 122 -130
3 61 -59
5 56 58

7 K 5
1 63 60
2 56 -52
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4 13 8

8 K 5
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2 104 108
3 83 82

9 K 5
1 43 -46

0 K 6
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4 37 -31
5 36 -35
6 121 -140

1 K 6
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1 111 113
2 68 -75
3 118 112
4 24 -22
5 20 -19
6 68 71

2 K 6
0 226 -204
1 168 -164
2 20 -14
3 23 -21
4 109 115
5 76 76
6 34 37

3 K 6
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1 195 -217
2 68 71
3 118 -128
4 23 16
5 69 69
6 67 -71

4 K 6
0 64 54
1 106 101
2 67 77
3 17 15
4 52 -48
5 51 -47
6 79 -91

5 K 6
0 87 82
1 42 32
2 59 -59
3 68 77
4 26 -25
5 20 9

6 K 6
0 72 -64
1 90 -84
2 59 -55
3 15 -14
4 59 59
5 40 42

7 K 6
0 51 -45
1 137 -138
2 40 42
3 89 -89
4 10 6

8 K 6
1 75 83
2 62 21
3 13 9

9 K 6
1 43 54

0 K 7
1 224 160*
2 128 119
3 138 -135
4 139 -160

5 27 -25
6 37 40

1 K 7
1 139 141
2 74 72
3 151 -132
4 54 48
5 28 -27
6 36 -35

2 K 7
1 53 -46
2 80 87
3 15 2
4 80 77
5 51 53
6 63 -59

3 K 7
1 149 -134
2 18 -9
3 136 160
4 88 -87
6 29 28

4 K 7
1 107 96
2 30 26
3 67 -70
4 108 -110
5 35 -33
6 38 44

5 K 7
1 104 96
2 80 84
3 74 -77
4 23 18
5 33 -31

6 K 7
1 81 -72
2 27 -15
3 62 57
4 99 96

7 K 7
1 102 -108
2 14 -6
3 122 127
4 51 -62

8 K 7
1 34 38
2 32 -29

0 K 8
1 122 -117
2 53 -48
3 78 -84
4 25 21
5 46 51
6 51 55

1 K 8
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1 108 -116
2 26 -20
3 30 -22
4 90 -101
5 60 58

2 K 8
0 107 -98
1 74 -73
2 66 66
3 79 78
4 16 17
5 71 68
6 60 -71

3 K 8
0 95 -81
1 126 111
2 14 -10
3 38 36
4 57 59
5 51 -53
6 23 25

4 K 8
0 55 47
1 38 -37
2 49 -53
3 70 -76

5 K 8
0 221 212
1 101 -96
2 30 -30
3 21 -15
4 99 -106
5 59 53

6 K 8
0 29 -22
1 25 22
2 43 39
3 59 61
4 14 -8

7 K 8
0 63 -59
1 73 72
2 15 -10
3 24 22

8 K 8
0 53 53
1 24 -20
2 33 42

0 K 9
1 58 -53
2 70 62
3 52 -45
4 49 -45
5 105 108

1 K 9
1 26 -23
2 168 -184
3 37 31
4 55 48
5 22 -18
6 30 32

2 K 9
1 14 -0
2 84 84
3 76 73
4 56 -56
5 90 -97
6 12 -11

3 K 9
1 34 -31
2 127 144
3 42 42
4 17 -12

4 K 9
1 47 -37
3 45 -40
5 92 92

5 K 9
1 50 -40
2 142 -163
3 61 60
4 58 54

6 K 9
1 28 17
2 17 10
3 54 51

7 K 9
1 25 -22
2 100 110
3 27 29

8 K 9
1 10 -15

0 K10
1 89 -89
2 82 -78
3 65 51
4 22 -12
5 66 69

1 K10
0 123 -149
1 74 -73
3 49 -44
4 72 66
5 34 26

2 K10
0 54 51
1 27 -23
2 33 26
3 81 -77
4 43 -45
5 23 -20

3 K10
0 179 175
1 128 138
2 44 -36
3 49 49
4 71 -75
5 61 -64

4 K10
0 41 29
1 38 -35
2 53 -55
3 58 54
5 34 42

5 K10
0 114 -100
1 35 -28
3 35 -33
4 44 47

6 K10
1 41 30
2 38 37
3 45 -49

7 K10
0 113 128
1 77 96
2 24 -25

0 K11
1 15 -15
2 17 17
3 54 51
4 99 98
5 39 -36

1 K11
1 106 -132
2 14 -8
3 110 109
4 33 20
5 29 27

2 K11
1 54 -39
2 21 -16
3 54 52
4 104 -115

3 K11
1 113 111
2 87 -83
3 99 -96
4 31 28
5 23 -27

4 K11
1 19 -4
3 28 21
4 80 96

5 K11
1 119 -112
2 55 -45
3 89 94
4 29 38

6 K11
1 24 -15
2 17 -17

7 K11
1 57 84*

In the subsequent cycles of anisotropic refinement, some reflections were seen to still suffer from errors which appeared to be greater than those in the data measurement and could be due to low precision in the absorption correc-

tion, to anisotropy in the secondary extinction or to primary extinction. For this reason 11 reflections were excluded from the final refinement. The R value converged to 0.084 (0.096 including all observed reflections).

The final positional and thermal parameters are given in Table 3 and the observed and calculated structure factors in Table 4. The calculated structure factors are based on atomic scattering factors given by Cromer and Waber [11] for tellurium and by Doyle and Turner [12] for copper and oxygen, the tellurium and copper values having been corrected for the real part of the anomalous scattering.[13] In the final cycles of refinement weights according to the formula $w=(20.0+|F_o|+0.01|F_c|^2+0.0001|F_o|^3)^{-1}$ were used.

Intensity corrections, Fourier summations and least squares refinements were performed with the programs DATAP2 [14] (modified for extinction correction), DRF [15] and LALS,[16] respectively. Interatomic distances and angles were obtained with the program DISTAN.[17]

DISCUSSION

Bond distances and angles for the oxygen coordination of the tellurium and oxygen atoms in $CuTeO_3$ are given in Table 5 (*cf.* also Figs. 1 and 2). Te_1 exhibits a pure three-fold pyramidal oxygen coordination, while Te_2 has in addition a fourth oxygen neighbour, about 0.4 Å more distant from Te_2 than the other three. This fourth oxygen atom is a member of the Te_1 oxygen pyramid, and Te_2O_6 units are thus formed. These units are connected by the copper atoms to form a three-dimensional network. Due to the strongly directed Te–O bonds, a rather open structure is formed, containing distinct tunnels visible in Fig. 3.

The four-coordinated Te_2 atom has all bonded atoms on the same side of a plane through itself, a phenomenon which has been found in two modifications of TeO_2 [18,19] and in other tellurium(IV) oxocompounds.[20] The three-fold

Table 5. Coordination distances (Å) and angles (°) in $CuTeO_3$. Notation in accordance with Figs. 1 and 2. Standard deviations in parentheses.

Te_1-O_4	1.86(2)	$O_1-Te_1-O_1'$	92.7(9)
Te_1-O_1 (2×)	1.89(2)	$O_1-Te_1-O_4$ (2×)	95.6(7)
(Te_1-O_3	2.71(2))		
(Te_1-O_2 (2×)	2.86(2))	$O_2-Te_2-O_2'$	105.7(1.1)
		$O_2-Te_2-O_3$ (2×)	86.0(7)
Te_2-O_2 (2×)	1.88(2)	$O_2-Te_2-O_4$ (2×)	91.7(7)
Te_2-O_3	1.96(2)	$O_3-Te_2-O_4$	176.3(8)
Te_2-O_4	2.32(2)	O_1-Cu-O_1'	78.4(7)
(Te_2-O_1 (2×)	3.16(2))	O_1-Cu-O_2	108.7(7)
		O_1-Cu-O_3	153.0(7)
$Cu-O_1$	1.94(2)	O_1-Cu-O_4	87.6(7)
$Cu-O_2$	1.97(2)	$O_1'-Cu-O_2$	154.2(8)
$Cu-O_1'$	1.97(2)	$O_1'-Cu-O_3$	87.0(8)
$Cu-O_3$	1.98(1)	$O_1'-Cu-O_4$	117.4(7)
$Cu-O_4$	2.38(2)	O_2-Cu-O_3	94.7(8)
($Cu-O_2'$	3.33(2))	O_2-Cu-O_4	88.2(7)
		O_3-Cu-O_4	79.1(7)

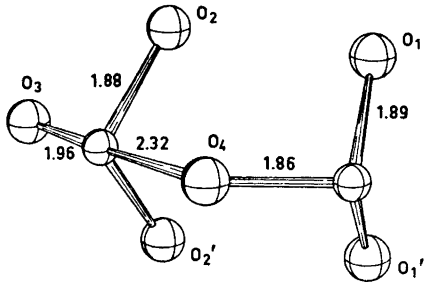

Fig. 1. Configuration of the Te_2O_6 subunit, drawn with the program ORTEP.[25]

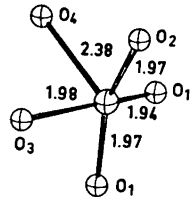

Fig. 2. The Cu(II) coordination.

pyramidal configuration of Te_1, with Te – O bond distances of 1.86 – 1.89 Å, is quite similar to the arrangement in $ZnTeO_3$ [3] and $CuTeO_3.2H_2O$ [4] in which there are Te – O distances of 1.86 – 1.89 Å and 1.81 – 1.89 Å, respectively. The O – Te – O bond angles are also of the same order of magnitude, $CuTeO_3.2H_2O$ having an average value of 99° which compares reasonably with the corresponding value of 94° found for Te_1 in $CuTeO_3$. However, in spite of the similar chemical composition of $ZnTeO_3$, $CuTeO_3.2H_2O$ and $CuTeO_3$, only $CuTeO_3$ contains the 3+1 coordination, the weaker Te – O interaction having a bond distance of 2.32 Å. This intermediate between three-

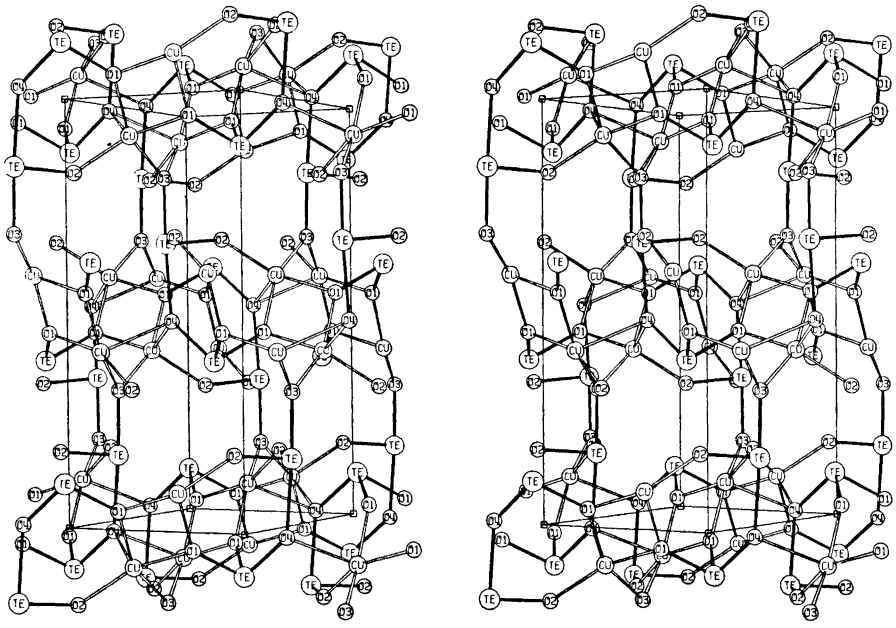

Fig. 3. Stereoscopic view of part of the $CuTeO_3$ structure (ORTEP [25]).

and four-fold coordination has been found in some other, more condensed tellurites, for example in $Zn_2Te_3O_8$ [21] and in (Mn,Ca,Zn)Te_2O_5 (denningite) [22] where the corresponding distances are 2.41 and 2.36 Å, respectively. In these two structures, the weak Te – O bonds form links in infinite Te – O chains.[20]

A tellurium-oxygen arrangement more similar to that in $CuTeO_3$ has been found in a recent investigation of $Fe_2(TeO_3)_2SO_4.3H_2O$ (poughite) [23] which also contains Te_2O_6 units. The shorter Te – O bonds in this compound, ranging from 1.85 – 1.99 Å and the intermediate bond of 2.38 Å, as well as most of the O – Te – O angles are of the same orders of magnitude as in $CuTeO_3$. The most marked difference is that the weakly bonded oxygen atom (O(7) in Ref. 23) is situated as close as 2.44 Å from the nearest oxygen atom (O(3) in Ref. 23), both coordinated to the same tellurium atom (Te(2)) and the angle O(3) – Te(2) – O(7) is only 68°, whereas in $CuTeO_3$ the corresponding values are 3.03(5) Å and 86°, respectively. These differences are due to the O(3) position in poughite, indicating appreciable strain in the oxygen coordination of Te(2). However, O(3) also is a member of both the Fe(1) and Fe(2) coordination octahedra, which might explain the deviation from the results in $CuTeO_3$.

The Cu(II) coordination is five-fold (*cf.* Fig. 2 and Table 5). The four closer oxygen atoms (1.94 – 1.98 Å) deviate appreciably from a planar configuration, and, taking into account the fifth oxygen atom (Cu – O = 2.38 Å), the coordination figure might be described as a distorted trigonal bipyramid. A similar arrangement, with one longer Me(II) – O distance, was found around Zn(II) in $ZnTeO_3$ [3] (1.96, 2.00, 2.02, 2.11 and 2.27 Å). A 4 + 1 coordination was also found in both $CuSeO_3.2H_2O$ [5] and $CuTeO_3.2H_2O$ [4] (Cu – O distances of 1.94 – 1.98 and 2.27 Å in $CuSeO_3.2H_2O$ and of 1.79 – 1.99 and 2.35 Å in $CuTeO_3.2H_2O$), but in these two structures the presence of water molecules permits the copper atom to coordinate its four nearest neighbours in a more regular way, with a smaller deviation from the expected planarity.

The lengths of the four shorter Cu – O bonds in $CuTeO_3$ are in good agreement with the values found in CuO (1.951 – 1.961 Å).[24] The fifth bond of 2.38 Å in $CuTeO_3$ also seems reasonable in comparison with CuO where the two more distant oxygen atoms completing a distorted octahedron are at distances of 2.78 Å.

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