

Short Communications

On the Crystal Structures of CuTeO₃ and CuTe₂O₅

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Single crystal structure investigations of CuTeO₃ and CuTe₂O₅ have been started. The crystals were synthesized by Moret, Philippot and Marin,¹ who also determined the unit cell dimensions:

CuTeO₃ - Orthorhombic (*P2₁nb* or *Pmnb*)
with $a = 7.604$, $b = 12.705$,
 $c = 5.837$ Å and $Z = 8$;

CuTe₂O₅ - Monoclinic (*P2₁/c*) with
 $a = 6.869$, $b = 9.324$, $c = 7.608$ Å,
 $\beta = 109.08^\circ$ and $Z = 4$.

For both structures Weissenberg equi-inclination data have been collected, and a total of 546 and 572 independent reflections have been measured for CuTeO₃ and CuTe₂O₅, respectively. The tellurium positions have been deduced from three-dimensional Patterson functions (*cf.* Tables 1 and 2), and for CuTeO₃ the copper and oxygen positions (Table 2) have also been determined from successive electron density calculations.

In the CuTeO₃ structure there are pyramidal TeO₃ groups with Te-O distances of 1.86-1.96 Å. The copper atom is irregularly coordinated by five oxygen atoms, four of which are nearly equi-distant (1.94-1.98 Å), the fifth bond being weaker (2.27 Å). The coordination of the metal atoms in CuTeO₃ is similar to that found in ZnTeO₃,² while the mode of connection of the TeO₃ and Me^{II}O₅ groups to form a

Table 1. Tellurium positions in CuTe₂O₅ (*P2₁/c*).

	<i>x</i>	<i>y</i>	<i>z</i>
Te ₁	0.38	0.30	0.32
Te ₂	0.90	0.18	0.32

Table 2. Atomic positions in CuTeO₃ (*Pmcn*).^a

	<i>x</i>	<i>y</i>	<i>z</i>
Te ₁	1/4	0.171	0.114
Te ₂	3/4	0.104	0.163
Cu	0.546	0.161	0.411
O ₁	0.427	0.340	0.048
O ₂	0.443	0.410	0.325
O ₃	3/4	0.108	0.318
O ₄	3/4	0.429	0.482

^a $a = 7.604$, $b = 5.837$ and $c = 12.705$ Å.
General equivalent positions
 $\pm(x, y, z)$; $\pm(1/2+x, 1/2+y, 1/2-z)$;
 $\pm(1/2+x, -y, -z)$; $\pm(x, 1/2-y, 1/2+z)$.

three-dimensional network is different in the two compounds.

The structure determinations of CuTeO₃ and CuTe₂O₅ are in progress, and detailed descriptions will follow.

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1. Moret, J., Philippot, E. and Maurin, M. *Compt. Rend. C* 269 (1969) 123.
2. Hanke, K. *Naturwiss.* 54 (1967) 199.

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