

Cu₂CoTeO₆**Richard Becker^{a*} and Helmuth Berger^b**^aInorganic Chemistry, Stockholm University, S-106 91 Stockholm, Sweden, and ^bInstitut de Physique de la Matière Complexe, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

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Key indicatorsSingle-crystal X-ray study
T = 292 K
Mean $\sigma(e-O)$ = 0.001 Å
Disorder in main residue
R factor = 0.014
wR factor = 0.043
Data-to-parameter ratio = 14.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Single crystals of dicopper(II) cobalt(II) tellurium(VI) hexoxide, Cu₂CoTeO₆, were synthesized from a molten TeO₂ flux. The structure is of the bixbyite type with approximately cubic close-packed O atoms with Te^{VI}, Cu^{II} and Co^{II} present at $\frac{2}{3}$ of the octahedral sites.

Comment

The crystal structure of Cu₃TeO₆ has been known since 1968 when Hostachy and Coing-Boyat first solved the structure from powder data (Hostachy & Coing-Boyat, 1968). Falck *et al.* (1978) later refined the structure from single-crystal data. Cu₃TeO₆ crystallizes in the cubic space group *Ia* $\bar{3}$ with a bixbyite type structure. Later work has involved replacing some of the Cu with other transition metals while retaining the same structure type and several such compounds have been found, *e.g.* Cu_{1.5}Zn_{1.5}TeO₆ and Cu_{1.5}Co_{1.5}TeO₆ (Müller-Buschbaum & Wulff, 1998), and Cu₂NiTeO₆ (Wedel *et al.*, 2001). Cu₃TeO₆ has gained interest from a magnetic-properties point of view and Herak *et al.* (2005) have reported a novel magnetic lattice, a three-dimensional spin web, in Cu₃TeO₆. It can be assumed that the introduction of a different transition metal into Cu₃TeO₆ might prove valuable to the understanding of this novel magnetic lattice type. The magnetically more complex Co^{II} has been introduced into the system and Co₃TeO₆ has been found (Becker *et al.*, 2006). This compound has a monoclinic structure with mixed coordinations for Co^{II}. Further investigations of the Cu_{3-x}Co_xTeO₆

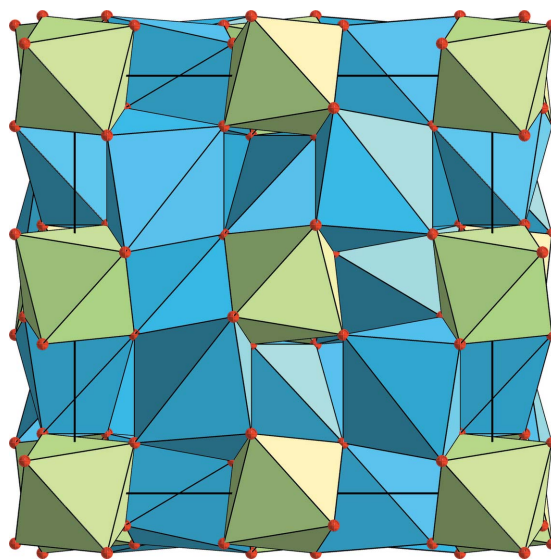
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Figure 1
The structure of (I), viewed down [100]. Key: green octahedra TeO₆ and blue octahedra (Cu/Co)O₆.

system led to the title compound $\text{Cu}_2\text{CoTeO}_6$, (I).

The structure of (I) is isostructural with Cu_3TeO_6 and is of the bixbyite type that is adopted by e.g. $(\text{Fe},\text{Mn})_2\text{O}_3$ (Pauling & Shappell, 1930; Dachs, 1956) and $\alpha\text{-Mn}_2\text{O}_3$ (Hase, 1963). The O atoms are approximately cubic close-packed and the Cu and Co (*M*) and Te atoms occupy some of the octahedral sites. The TeO_6 octahedron is slightly distorted but the MO_6 octahedron is highly distorted, with four shorter *M*–O bonds forming a square plane and two significantly longer *M*–O distances. These O atoms should ideally be positioned directly opposite each other, but the O–*M*–O angle is as low as $132.91(8)^\circ$.

The structure consists of a network of MO_6 octahedra connected *via* shared edges and corners. The Te atoms are positioned in octahedral positions in the MO_6 octahedra network, so that no TeO_6 octahedron shares a common oxygen with another TeO_6 octahedron, but solely with MO_6 octahedra (Fig. 1).

The single transition metal position in $\text{Cu}_2\text{CoTeO}_6$ is $\frac{2}{3}$ occupied by Cu and $\frac{1}{3}$ by Co. The occupancy was refined with *SHELXL97* (Sheldrick, 1997) and has been confirmed using the program *JANA2000* (Petříček & Dusek, 2000), as well as through EDS.

Experimental

Single crystals of $\text{Cu}_2\text{CoTeO}_6$ were grown from a molten TeO_2 flux. The starting materials were CuO (Alpha Aesar 99.99%), CoO (Alpha Aesar 99.999%) and TeO_2 (Acros 99%). The single crystals used in this study were grown from a mixture with the molar ratio CuO:CoO:TeO₂ 1:1:4. The powder was placed in an alumina crucible, which was covered with an alumina lid and heated in air to the reaction temperature of 1123 K at a rate of 100 K h⁻¹. The temperature was held at this level for 15 h, and the cooled to 673 K at a rate of 1 K h⁻¹, after which the sample was cooled quickly to room temperature by turning off the furnace. Black crystals were isolated from the flux matrix by washing with 1 M KOH solution.

Crystal data

$\text{Cu}_2\text{CoTeO}_6$	$D_x = 6.220 \text{ Mg m}^{-3}$
$M_r = 409.61$	Mo $K\alpha$ radiation
Cubic, $Ia\bar{3}$	$\mu = 19.87 \text{ mm}^{-1}$
$a = 9.5677(5) \text{ \AA}$	$T = 292(3) \text{ K}$
$V = 875.84(8) \text{ \AA}^3$	Block, black
$Z = 8$	$0.06 \times 0.05 \times 0.05 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur CCD diffractometer	7504 measured reflections
ω scans	280 independent reflections
Absorption correction: numerical (<i>CrysAlis RED</i> ; Oxford Diffraction, 2005)	278 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.218$, $T_{\max} = 0.294$	$R_{\text{int}} = 0.043$
	$\theta_{\max} = 33.2^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.014$
 $wR(F^2) = 0.043$
 $S = 1.75$
 280 reflections
 19 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0195P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.77 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.87 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.00185 (16)

Table 1

Selected bond lengths (Å).

Te1–O1	1.9332 (13)	Cu1–O1 ⁱⁱⁱ	1.9608 (15)
Te1–O1 ⁱ	1.9335 (13)	Cu1–O1 ^{iv}	2.0481 (15)
Te1–O1 ⁱⁱ	1.9339 (13)	Cu1–O1 ^v	2.3400 (15)

Symmetry codes: (i) z, x, y ; (ii) y, z, x ; (iii) $-x, -y, -z$; (iv) $y - \frac{1}{2}, -z - \frac{1}{2}, -x$; (v) $-z - \frac{1}{2}, x - \frac{1}{2}, y$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2005); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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