

YCu(TeO₃)₂(NO₃)(H₂O)₃: a novel layered telluriteStuart J. Mills,^{a*} Maja A. Dunstan^b and Andrew G. Christy^c

^aGeosciences, Museum Victoria, GPO Box 666, Melbourne 3001, Victoria, Australia, ^bSchool of Chemistry, University of Melbourne, Parkville 3010, Victoria, Australia, and ^cOcean and Climate Geoscience, Research School of Earth Sciences, Mills Rd, Australian National University, Canberra, ACT 2601, Australia. *Correspondence e-mail: smills@museum.vic.gov.au

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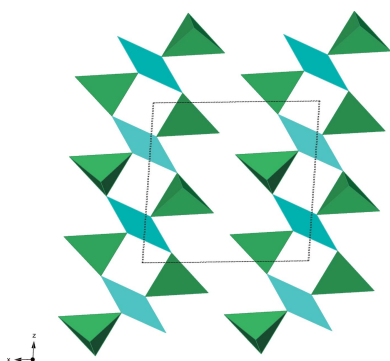
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A new hydrated yttrium copper tellurite nitrate, yttrium(III) copper(II) bis[trioxidotellurate(IV)] nitrate trihydrate, has been synthesized hydrothermally in a Teflon-lined autoclave and structurally determined using synchrotron radiation. The new phase is the first example containing yttrium, copper and tellurium in one structure. Its crystal structure is unique, with relatively strongly bound layers extending parallel to (020), defined by YO₈, CuO₄ and TeO₃ polyhedra, while the NO₃[−] anions and one third of the water molecules lie between those layers. The structural unit consists of [Cu₂(TeO₃)₄]^{4−} loop-branched chains of {Cu···Te···Cu···Te} squares running parallel to [001], which are linked further into layers only through Y(O,H₂O)₈ polyhedra. Weak ‘secondary’ Te bonds and O–H···O hydrogen-bonding interactions, involving water molecules and layer O atoms, link the layers and interlayer species. IR spectroscopic data are also presented.

1. Chemical context

Recent discoveries of a wide range of novel tellurium minerals have prompted numerous structural studies of tellurium oxysalts (Kampf *et al.*, 2013; Christy *et al.*, 2016a). As well as the characterization of these naturally occurring minerals, various syntheses have also been undertaken as part of this ongoing study, yielding an array of new structures, including that of novel Na₁₁H[Te(OH)₃]₈[SO₄]₁₀(H₂O)₁₃ (Mills *et al.*, 2016). Several tellurium oxide species with various yttrium oxide polyhedra present in the structure have been synthesized in the past, including compounds with both Te^{IV} and Te^{VI} atoms. Tellurium is stable in numerous oxidation states and shows large diversity in bonding (Christy & Mills, 2013). Its +IV and +VI oxidation states are of greatest interest in relation to naturally occurring weathering products of minerals, and are able to form a wide variety of oxide polyhedra, with TeO₃^{2−} most prevalent (Song *et al.*, 2014). The TeO₃^{2−} anion shows a wide variety of connectivities, with three oxido ligands and the 5s² electron lone pair occupying the vertices of the distorted polyhedra, and are found in a variety of layer and chain structures in inorganic compounds (Johansson & Lindqvist, 1978). This is demonstrated in compounds such as NaYTe₄O₁₀ with YO₈ and TeO₄ polyhedra, KY(TeO₃)₂ and RbY(TeO₃)₂ with YO₆ octahedra and trigonal-pyramidal TeO₃^{2−} anions, CsYTe₃O₈ with YO₆ and TeO₄ polyhedra (Kim *et al.*, 2014), as well as yttrium tellurium oxides with Te^{VI} atoms (Kasper, 1969; Höss & Schleid, 2007; Noguera *et al.*, 2012). As a consequence of this range of chemistry, tellurium is the most anomalously diverse element found in minerals



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Table 1
Bond-valence sums (in valence units) for $\text{YCu}(\text{TeO}_3)_2(\text{NO}_3)(\text{H}_2\text{O})_3$.

	Y1	Cu1	Te1	Te2	N1	H11	H12	H21	H22	H31	H32	Σ	$\Sigma(\text{excluding H})$
O1	0.401	0.544, 0.047	1.128									2.12	2.12
O2	0.478, 0.275		1.145	0.130								2.03	2.03
O3		0.436	1.208	0.173					0.232			2.05	1.82
O4	0.399	0.534, 0.046		1.148			0.041					2.17	2.13
O5	0.481, 0.316	0.421	0.118	1.165								2.08	2.08
O6			0.183	1.179			0.279					2.06	1.78
O7			0.156		1.562							1.72	1.72
O8				0.156	1.609			0.068		0.047		1.88	1.77
O9					1.712						0.062, 0.036	1.81	1.71
OW1	0.384					0.755	0.755					1.89	0.38
OW2	0.389							0.771	0.769			1.93	0.39
OW3						0.224		0.110		0.743	0.761	1.84	0.00
Σ	3.12	2.03	3.93	3.94	4.88	0.98	1.08	0.95	1.00	0.79	0.86		

compared to its scarcity in the earth's crust (Christy, 2015). Many copper-containing tellurium oxides have been successfully synthesized (Feger *et al.*, 1999; Koteswararao *et al.*, 2013; Sedello & Müller-Buschbaum, 1996), and copper is also present in many tellurium-containing minerals; indeed, out of the unusually large inventory of tellurium secondary minerals at Otto Mountain, the majority contains copper (Christy *et al.*, 2016a). Despite this, there are very few synthetic rare earth copper tellurium oxides known, and to the best of our knowledge a compound containing all three of copper, yttrium and tellurium has not been characterized so far. Although layered structures with interstitial ions are common for Te^{IV} compounds, nitrate is found as an anion in very few, which motivates the use of metal nitrates in the synthesis of novel tellurium oxides. The only other compounds with simple tellurite and nitrate anions whose structures have been reported to date are the layered compounds $\text{Ca}_6(\text{TeO}_3)_5(\text{NO}_3)_2$ and $\text{Ca}_5(\text{TeO}_3)_4(\text{NO}_3)_2(\text{H}_2\text{O})_2$ (Stöger & Weil, 2013). Nitrates of polymerized Te(IV) complexes are also known. The compound $\text{AgTeO}_2(\text{NO}_3)$ (Olsson *et al.*, 1988) contains an electrically neutral $[\text{Te}_2\text{O}_4]^0$ chain (Christy *et al.*, 2016b), while $[\text{Te}_2\text{O}_3\text{OH}](\text{NO}_3)$ contains a cationic $[\text{Te}_2\text{O}_3\text{OH}]^+$ layer (Anderson *et al.*, 1980; Christy *et al.*, 2016b).

2. Structural commentary

Bond-valence sums are given in Table 1. In general, the bond-valence data of Table 1 were calculated using the bond-valence parameters of Brown & Altermatt (1985), except that the Te—O data were from Mills & Christy (2013). However, Brown (2009) noted that no single pair of r_0 and b values is adequate for O—H bonds, since O···O repulsion increases the length of weak O—H bonds relative to strong ones. Here, the parameterization of Yu *et al.* (2006) was used, with $r_0 = 0.79$ Å for bond valence < 0.5 valence units, $r_0 = 1.409$ Å for bond valence > 0.5 v.u., and $b = 0.37$ Å in both cases.

The structure of the title compound is strongly layered. Layers parallel to (020) are defined by YO_8 , CuO_4 and TeO_3 polyhedra, while NO_3^- anions and one third of the water molecules (OW1) lie between those layers. Tellurite and nitrate anions (involving atoms O1–O9) are clearly distin-

guished from water molecules OW1–OW3 by their bond-valence sums (Table 1). Within the layers, Y is eightfold coordinated in a distorted snub disphenoidal (triangular dodecahedral) arrangement by $6 \times \text{O}^{2-}$ and $2 \times \text{H}_2\text{O}$ at 2.290 (3)–2.497 (3) Å. Cu is in square-planar coordination, with four close oxygen neighbours at 1.904 (3)–1.999 (3) Å. Two more oxygen ligands at 2.811 (4) and 2.817 (4) Å complete an octahedron that is very elongated due to the Jahn-Teller distortion. Te1 is trigonal-pyramidally coordinated by three oxygen atoms at 1.883 (3)–1.911 (3) Å. Three 'secondary bonds' to O atoms at 2.657 (3)–2.837 (3) Å complete a polyhedron that can be described as an octahedron that is very distorted due to the lone-pair stereoactivity. Te2 has very similar coordination, with three primary Te—O bonds of 1.893 (3)–1.905 (3) Å and three secondary bonds of 2.681 (4)–2.798 (3) Å. In each case, two of the secondary bonds provide additional bracing within the $\{\text{Y}\cdots\text{Cu}\cdots\text{Te}\}$ layer, while the third is to a nitrate oxygen (Te1—O7 and Te2—O8, both $\simeq 2.72$ Å), and thus provides weak bridging between the layers and interlayer species. The nitrate oxygen atom O9 makes a seventh very distant ligand for both Te1 [3.231 (4) Å] and Te2 [3.350 (4) Å], further than the shortest Te···Cu distances and with bond valences < 0.05 valence units, using the parameters of Mills & Christy (2013).

The identification and classification of a strongly bonded 'structural unit' (Hawthorne, 2014) in the structure of this compound depends crucially on which bonds are regarded as strong enough to define such a unit. The classification of Te oxycompound structures by Christy *et al.* (2016b) in general used thresholds of about 2.45 Å for Te—O and 2.20 Å for Cu—O bonds, while no bonds to 8-fold coordinated cations were considered to be part of the structural unit. The same criteria applied to the current structure would regard the CuO_4 squares as isolated from one another, although inclusion of the long Cu—O bonds would link CuO_{4+2} polyhedra to form *trans* edge-sharing chains parallel to [001]. Without the long bonds, CuO_4 squares are linked to their neighbours most strongly *via* TeO_3 pyramids, to produce loop-branched chains $[\text{Cu}_2(\text{TeO}_3)_4]^{4-}$ of $\{\text{Cu}\cdots\text{Te}\cdots\text{Cu}\cdots\text{Te}\}$ squares running parallel to [001] (Fig. 1). These chains are the structural units, since they are linked further into layers only through

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
OW1—H11···OW3	0.89 (3)	1.96 (3)	2.854 (6)	174 (7)
OW1—H12···O6 ⁱ	0.89 (3)	1.88 (4)	2.729 (5)	157 (7)
OW2—H21···O8 ⁱ	0.89 (3)	2.41 (6)	3.074 (5)	132 (6)
OW2—H21···OW3 ⁱⁱ	0.89 (3)	2.22 (5)	2.949 (6)	139 (6)
OW2—H22···O3	0.89 (3)	1.95 (5)	2.745 (5)	149 (7)
OW3—H31···O7	0.90 (3)	1.97 (4)	2.834 (7)	162 (9)
OW3—H31···O8 ⁱⁱⁱ	0.90 (3)	2.53 (8)	3.141 (7)	126 (7)
OW3—H32···O9 ^{iv}	0.89 (3)	2.49 (4)	3.360 (7)	166 (9)
OW3—H32···O9 ^v	0.89 (3)	2.64 (9)	3.253 (8)	127 (8)

Symmetry codes: (i) $x - 1, -y + \frac{1}{2}, z - \frac{3}{2}$; (ii) $-x, -y + 1, -z$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (iv) $x - 1, y, z$; (v) $-x, -y + 1, -z + 1$.

Y(O,H₂O)₈ polyhedra (Fig. 2). It is noteworthy that this chain is similar in topology but not in geometrical configuration to the structural unit of Dy[CuCl(TeO₃)₂] and its Er—Cl and Er—Br analogues (Shen & Mao, 2005). However, in the current compound, the {Cu···Te} squares are non-planar, so that the chain periodicity is doubled, and Cu does not have chloride as an additional ligand. Furthermore, in the structures of the compounds of Shen and Mao (2005), rare earth cations link the chains into a three-dimensional framework rather than into layers.

H11, H12, H22 and H31 were found to make relatively strong hydrogen bonds (Table 2) to respectively OW3, O6, O3 and O7 at distances between 1.88–1.96 Å. H12 and H31 have additional acceptor O atoms at greater distances, respectively O4 at 2.59 Å and O8 at 2.54 Å. The remaining H atoms each have two oxygen neighbours at greater distances, suggesting weak bifurcated hydrogen bonding: OW3 at 2.23 Å and O8 at 2.40 Å for H21, and O8 at 2.44 Å, O9 at 2.64 Å for H32.

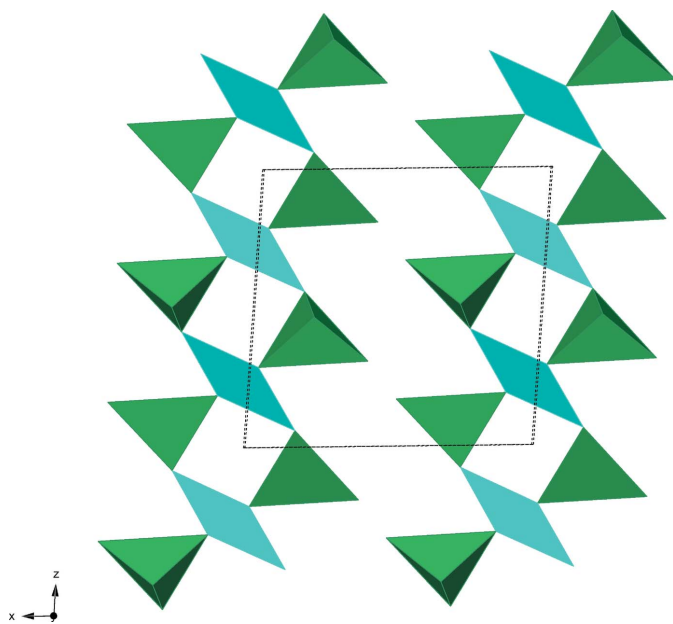


Figure 1
View in polyhedral mode of the [Cu₂(TeO₃)₄]⁴⁻ loop-branched chains running parallel to [001]. CuO₄ polyhedra are cyan, TeO₃ polyhedra are green

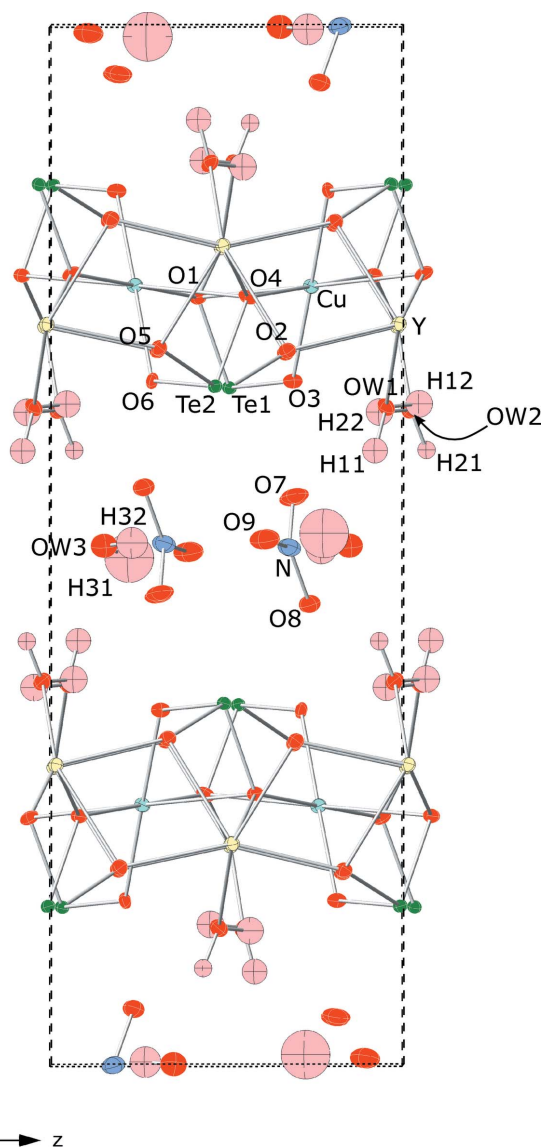


Figure 2
The crystal structure of YCu(TeO₃)₂(NO₃)(H₂O)₃ viewed down [100]. O atoms are red, Y yellow, Cu cyan, Te green, N light-blue and O atoms of water molecules pink. Displacement ellipsoids are drawn at the 50% probability level.

The layers of the structure are linked by only weak bonds. The bridges Te1···O7—N—O8···Te2 mentioned above have Te···O ≈ 2.72 Å, implying a bond of 0.15 valence units (Mills & Christy, 2013). The hydrogen bonds in the bridges OW1—H11···OW3···H21—OW2 are of comparable bond valence.

It is noteworthy that the IR spectrum shows three distinct O—H bands at 3460, 3145 and 2900 cm⁻¹. According to Libowitzky (1999), this would be typical for O—H···O distances of ~ 2.83, 2.69 and 2.63 Å. The first two of these are broadly consistent with the O···O distances for the strongest hydrogen bonds indicated by the refinement: OW1—H12···OW3 = 2.85 Å, OW2—H12···O3 = 2.74 Å and OW1—H11···O6 = 2.73 Å. However, the band at 2900 cm⁻¹ is lower in frequency than would be expected.

Table 3
IR band assignments (cm⁻¹) for YCu(TeO₃)₂(NO₃)(H₂O)₃.

Absorption bands	Assignment
3460 _w	O—H stretch
3145 _w	O—H stretch
~2900 _w	O—H stretch
1755	H—O—H bend
1645	H—O—H bend
1605	H—O—H bend
1345	ν_3 antisymmetric stretch NO ₃ ⁻
1044	ν_1 symmetric stretch NO ₃ ⁻
734	ν_1 (TeO ₃) ²⁻ symmetric stretch
636	ν_3 (TeO ₃) ²⁻ antisymmetric stretch
547	M—O lattice modes
447	M—O lattice modes

3. Spectroscopy

The infrared spectrum was obtained using a Bruker Alpha FTIR with a diamond Attenuated Total Reflectance attachment (ATR), DTGS (Deuterated Triglycine Sulfate) detector, 4 cm⁻¹ resolution and 4000–450 cm⁻¹ range. The samples were placed on the ATR crystal and pressure exerted by screwing the pressure clamp onto the sample to ensure maximum contact with the ATR crystal. 128 scans were taken for each item and co-added. Band assignments are consistent with those given in Kampf *et al.* (2013). Numerical values of the spectrum and assignments of the vibration bands are given in Table 3; the spectrum is deposited as a supplementary figure.

4. Synthesis and crystallization

Dark blue prisms of YCu(TeO₃)₂(NO₃)(H₂O)₃ were synthesized hydrothermally. For the synthesis, Y(NO₃)₃·6H₂O (Aldrich, 99.8%), Cu(NO₃)₂·3H₂O (Sigma–Aldrich ≥99%) and Te 200 mm mesh (Aldrich, 99.8%) were used as starting materials. A 1:1:1 molar ratio of the reagents in 20 ml water was reacted in a Teflon autoclave bomb at 473 K for 3 days. Crystals of YCu(TeO₃)₂(NO₃)(H₂O)₃ were separated manually from a blue powder of undetermined composition in a few percent yield. Several unsuccessful attempts were made to synthesize YCu(TeO₃)₂(NO₃)(H₂O)₃ from a stoichiometric mixture of the reagents, using the molar ratio 1:1:2. We also were unsuccessful in producing new compounds, with the same structure type or not, using La, Ce, Nd or Gd in place of Y.

5. Refinement

Single crystal X-ray diffraction experiments were carried out on the micro-focus macromolecular beam line MX2 of the Australian Synchrotron. Details of data collection and structure refinement are provided in Table 4. Hydrogen atoms H11, H12 and H21 were located during refinement as difference peaks of about one e⁻ / Å³ occurring at a distance of ca. 0.9–1.0 Å from their nearest oxygen atom. In all cases, short O—H bonds were directed towards another oxygen atom, indicating

Table 4
Experimental details.

Crystal data	YCu(TeO ₃) ₂ (NO ₃)(H ₂ O) ₃
Chemical formula	619.71
<i>M_r</i>	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Crystal system, space group	100
Temperature (K)	7.2560 (15), 20.654 (4), 7.0160 (14)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	94.63 (3)
β (°)	1048.0 (4)
<i>V</i> (Å ³)	4
<i>Z</i>	Synchrotron, $\lambda = 0.71073$ Å
Radiation type	13.06
μ (mm ⁻¹)	0.02 × 0.02 × 0.01
Crystal size (mm)	
Data collection	
Diffractometer	ADSC Quantum 315r detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2001)
<i>T</i> _{min} , <i>T</i> _{max}	0.295, 0.433
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	20336, 2901, 2810
<i>R</i> _{int}	0.054
(sin θ/ <i>λ</i>) _{max} (Å ⁻¹)	0.704
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.033, 0.074, 1.14
No. of reflections	2901
No. of parameters	173
No. of restraints	6
H-atom treatment	Only H-atom coordinates refined
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	1.45, -1.56

Computer programs: local program, *XDS* (Kabsch, 2010), *XPREP* (Bruker, 2001), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *CrystalMaker* (Palmer, 2009) and *publCIF* (Westrip, 2010).

the existence of hydrogen bonds. Positions were estimated for the remaining hydrogen atoms, assuming water molecule O—H distance near 0.9 Å, H—O—H bond angle near 104°, that O—H vectors were directed to make hydrogen bonds to nearby oxygen atoms, if possible, and that the arrangement of O—H and O···H around OW3 was approximately tetrahedral. In all cases, residuals of > 0.6 electrons were found close to the expected positions, that could be identified with the H atoms. H positions were finally included in the refinement, assuming full occupancy, isotropic displacement parameters were fixed to 1.5× of their corresponding O atom and the O—H distance was restrained at 0.90 (3) Å.

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YCu(TeO₃)₂(NO₃)(H₂O)₃: a novel layered tellurite

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Computing details

Data collection: local program; cell refinement: *XDS* (Kabsch, 2010); data reduction: *XPREP* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (Palmer, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Yttrium(III) copper(II) bis[trioxidotellurate(IV)] nitrate trihydrate

Crystal data

YCu(TeO₃)₂(NO₃)(H₂O)₃

$M_r = 619.71$

Monoclinic, $P2_1/c$

$a = 7.2560$ (15) Å

$b = 20.654$ (4) Å

$c = 7.0160$ (14) Å

$\beta = 94.63$ (3)°

$V = 1048.0$ (4) Å³

$Z = 4$

$F(000) = 1124$

$D_x = 3.928$ Mg m⁻³

Synchrotron radiation, $\lambda = 0.71073$ Å

Cell parameters from 20243 reflections

$\theta = 2.8$ – 30.0 °

$\mu = 13.06$ mm⁻¹

$T = 100$ K

Prism, dark blue

$0.02 \times 0.02 \times 0.01$ mm

Data collection

ADSC Quantum 315r detector
diffractometer

Radiation source: synchrotron
 φ scan

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.295$, $T_{\max} = 0.433$

20336 measured reflections

2901 independent reflections

2810 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.054$

$\theta_{\max} = 30.0$ °, $\theta_{\min} = 2.8$ °

$h = -10$ → 10

$k = -29$ → 29

$l = -9$ → 9

360 standard reflections every 1 reflections

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.074$

$S = 1.14$

2901 reflections

173 parameters

6 restraints

Hydrogen site location: difference Fourier map

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + 11.0043P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.45$ e Å⁻³

$\Delta\rho_{\min} = -1.56$ e Å⁻³

Extinction correction: *SHELXL2014*
(Sheldrick, 2015),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0094 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	0.21415 (4)	0.34749 (2)	0.49104 (4)	0.00849 (9)
Te2	0.71124 (4)	0.15281 (2)	1.03341 (4)	0.00846 (9)
Y1	−0.03880 (6)	0.28786 (2)	0.01247 (6)	0.00865 (11)
Cu1	0.46115 (7)	0.24947 (2)	0.76001 (8)	0.00911 (12)
N1	0.8271 (7)	0.0010 (2)	1.1795 (7)	0.0209 (9)
O1	0.2531 (4)	0.26068 (15)	0.5797 (5)	0.0105 (6)
O2	0.0133 (4)	0.31345 (15)	0.3301 (5)	0.0106 (6)
O3	0.3929 (4)	0.34159 (15)	0.3116 (5)	0.0112 (6)
O4	0.6704 (4)	0.23870 (15)	0.9406 (5)	0.0114 (6)
O5	0.9077 (4)	0.18938 (15)	1.1933 (5)	0.0106 (6)
O6	0.5292 (5)	0.15853 (15)	1.2113 (5)	0.0099 (6)
O7	0.0622 (7)	0.45346 (18)	0.3091 (7)	0.0279 (10)
O8	0.8860 (6)	0.05534 (18)	1.2373 (6)	0.0233 (8)
O9	0.3327 (6)	0.49362 (19)	0.3909 (7)	0.0284 (9)
OW1	−0.2697 (5)	0.36731 (17)	0.0483 (5)	0.0134 (6)
H11	−0.266 (10)	0.4092 (16)	0.080 (10)	0.020*
H12	−0.360 (8)	0.364 (4)	−0.046 (8)	0.020*
OW2	0.1872 (5)	0.36858 (17)	−0.0246 (5)	0.0153 (7)
H21	0.155 (10)	0.407 (2)	−0.070 (10)	0.023*
H22	0.279 (8)	0.371 (4)	0.066 (8)	0.023*
OW3	−0.2844 (7)	0.5007 (2)	0.1525 (8)	0.0317 (10)
H31	−0.182 (9)	0.490 (4)	0.225 (12)	0.048*
H32	−0.374 (10)	0.503 (4)	0.232 (12)	0.048*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.00827 (14)	0.00782 (13)	0.00912 (16)	−0.00013 (8)	−0.00084 (9)	−0.00064 (9)
Te2	0.00858 (14)	0.00783 (14)	0.00876 (16)	0.00007 (8)	−0.00061 (9)	−0.00066 (9)
Y1	0.00832 (19)	0.00855 (19)	0.0089 (2)	0.00012 (13)	−0.00055 (14)	0.00008 (13)
Cu1	0.0081 (2)	0.0088 (2)	0.0100 (3)	−0.00025 (17)	−0.00157 (18)	0.00098 (18)
N1	0.027 (2)	0.0128 (19)	0.022 (2)	−0.0008 (16)	−0.0056 (18)	0.0026 (16)
O1	0.0103 (14)	0.0089 (13)	0.0119 (16)	0.0001 (11)	−0.0018 (11)	0.0007 (11)
O2	0.0089 (14)	0.0102 (14)	0.0125 (16)	−0.0020 (11)	−0.0009 (11)	0.0003 (11)
O3	0.0080 (14)	0.0096 (13)	0.0163 (17)	0.0003 (11)	0.0032 (12)	0.0002 (11)
O4	0.0098 (14)	0.0093 (13)	0.0147 (17)	0.0005 (11)	−0.0018 (12)	0.0038 (11)
O5	0.0109 (14)	0.0095 (13)	0.0109 (16)	−0.0014 (11)	−0.0015 (11)	−0.0007 (11)
O6	0.0115 (14)	0.0116 (14)	0.0067 (15)	0.0012 (11)	0.0017 (11)	−0.0014 (11)
O7	0.038 (2)	0.0108 (16)	0.032 (2)	−0.0057 (16)	−0.0148 (19)	0.0042 (15)

O8	0.034 (2)	0.0136 (16)	0.020 (2)	0.0006 (15)	-0.0072 (16)	-0.0014 (14)
O9	0.026 (2)	0.0194 (18)	0.038 (3)	0.0027 (15)	-0.0085 (18)	0.0027 (17)
OW1	0.0137 (15)	0.0128 (15)	0.0128 (17)	0.0022 (12)	-0.0036 (12)	-0.0031 (12)
OW2	0.0176 (16)	0.0140 (15)	0.0137 (18)	-0.0029 (13)	-0.0016 (13)	0.0024 (12)
OW3	0.039 (3)	0.025 (2)	0.031 (3)	0.0023 (19)	0.000 (2)	0.0002 (18)

Geometric parameters (Å, °)

Te1—O3	1.883 (3)	O2—Cu1 ⁱ	3.571 (3)
Te1—O2	1.905 (3)	O3—Cu1 ⁱ	1.986 (3)
Te1—O1	1.911 (3)	O3—Te2 ⁱ	2.681 (3)
Te1—O6 ⁱ	2.657 (3)	O4—Y1 ^{ix}	2.359 (3)
Te1—O7	2.722 (4)	O4—Cu1 ⁱⁱⁱ	2.817 (4)
Te1—O5 ⁱⁱ	2.837 (3)	O4—Te2 ⁱ	3.661 (3)
Te2—O6	1.893 (3)	O4—Te1 ⁱⁱⁱ	3.801 (3)
Te2—O5	1.898 (3)	O4—Y1 ^{iv}	3.847 (4)
Te2—O4	1.905 (3)	O5—Y1 ^x	2.290 (3)
Te2—O3 ⁱⁱⁱ	2.681 (4)	O5—Y1 ^{ix}	2.445 (3)
Te2—O8	2.723 (4)	O5—Te1 ^{iv}	2.837 (3)
Te2—O2 ^{iv}	2.798 (3)	O5—Cu1 ⁱⁱⁱ	3.543 (3)
Y1—O5 ^v	2.290 (3)	O6—Cu1 ⁱⁱⁱ	1.999 (3)
Y1—O2	2.292 (3)	O6—Te1 ⁱⁱⁱ	2.657 (3)
Y1—O1 ⁱ	2.357 (3)	O6—Y1 ^x	3.801 (3)
Y1—O4 ^{vi}	2.359 (3)	O7—N1 ^{xi}	1.267 (6)
Y1—OW2	2.367 (4)	O7—Te2 ⁱⁱ	3.798 (5)
Y1—OW1	2.373 (3)	O8—Te1 ^{iv}	3.653 (5)
Y1—O5 ^{vi}	2.445 (3)	O8—Y1 ^x	3.787 (4)
Y1—O2 ⁱ	2.497 (3)	O9—N1 ^{xi}	1.233 (6)
Cu1—O1	1.904 (3)	O9—Te2 ^{xi}	3.350 (4)
Cu1—O4	1.910 (3)	O9—Te2 ⁱ	4.153 (4)
Cu1—O3 ⁱⁱⁱ	1.986 (3)	OW1—Te2 ⁱⁱ	3.442 (4)
Cu1—O6 ⁱ	1.999 (3)	OW1—Cu1 ⁱⁱ	3.508 (4)
Cu1—O1 ⁱⁱⁱ	2.811 (4)	OW1—Te2 ^v	3.628 (4)
Cu1—O4 ⁱ	2.817 (4)	OW1—Cu1 ^{vi}	3.632 (4)
N1—O9 ^{vii}	1.233 (6)	OW1—H11	0.89 (3)
N1—O8	1.256 (6)	OW1—H12	0.89 (3)
N1—O7 ^{vii}	1.267 (6)	OW2—Te1 ^{xii}	3.447 (4)
N1—Te1 ^{vii}	3.394 (4)	OW2—Cu1 ^{xii}	3.574 (4)
O1—Y1 ⁱⁱⁱ	2.357 (3)	OW2—Cu1 ⁱ	3.639 (4)
O1—Cu1 ⁱ	2.811 (4)	OW2—H21	0.89 (3)
O1—Te1 ⁱⁱⁱ	3.679 (3)	OW2—H22	0.89 (3)
O1—Te2 ⁱ	3.811 (3)	OW3—Te1 ^{xiii}	4.018 (5)
O1—Y1 ^{viii}	3.881 (4)	OW3—Te2 ⁱⁱ	4.148 (5)
O2—Y1 ⁱⁱⁱ	2.497 (3)	OW3—H31	0.90 (3)
O2—Te2 ⁱⁱ	2.798 (3)	OW3—H32	0.89 (3)
O3—Te1—O2	96.62 (15)	Cu1 ⁱ —O3—Te2 ⁱ	86.04 (11)
O3—Te1—O1	93.73 (14)	Te1—O3—Cu1	60.91 (10)

O2—Te1—O1	86.15 (14)	Cu1 ⁱ —O3—Cu1	69.36 (10)
O3—Te1—O6 ⁱ	77.24 (13)	Te2 ⁱ —O3—Cu1	58.36 (7)
O2—Te1—O6 ⁱ	155.35 (12)	Te1—O3—Y1	78.82 (10)
O1—Te1—O6 ⁱ	70.67 (12)	Cu1 ⁱ —O3—Y1	80.15 (10)
O3—Te1—O7	90.77 (15)	Te2 ⁱ —O3—Y1	165.46 (11)
O2—Te1—O7	75.93 (13)	Cu1—O3—Y1	111.74 (8)
O1—Te1—O7	161.92 (13)	Te2—O4—Cu1	115.38 (17)
O6 ⁱ —Te1—O7	127.41 (11)	Te2—O4—Y1 ^{ix}	102.48 (14)
O3—Te1—O5 ⁱⁱ	157.99 (12)	Cu1—O4—Y1 ^{ix}	137.81 (17)
O2—Te1—O5 ⁱⁱ	66.69 (13)	Te2—O4—Cu1 ⁱⁱⁱ	83.55 (12)
O1—Te1—O5 ⁱⁱ	71.75 (12)	Cu1—O4—Cu1 ⁱⁱⁱ	93.83 (13)
O6 ⁱ —Te1—O5 ⁱⁱ	111.64 (10)	Y1 ^{ix} —O4—Cu1 ⁱⁱⁱ	108.82 (13)
O7—Te1—O5 ⁱⁱ	98.40 (13)	Te2—O4—Te2 ⁱ	144.76 (16)
O6—Te2—O5	96.67 (15)	Cu1—O4—Te2 ⁱ	61.40 (9)
O6—Te2—O4	94.00 (14)	Y1 ^{ix} —O4—Te2 ⁱ	77.07 (9)
O5—Te2—O4	85.42 (14)	Cu1 ⁱⁱⁱ —O4—Te2 ⁱ	130.56 (10)
O6—Te2—O3 ⁱⁱⁱ	76.45 (13)	Te2—O4—Te1 ⁱⁱⁱ	69.18 (9)
O5—Te2—O3 ⁱⁱⁱ	153.70 (12)	Cu1—O4—Te1 ⁱⁱⁱ	57.63 (9)
O4—Te2—O3 ⁱⁱⁱ	70.03 (12)	Y1 ^{ix} —O4—Te1 ⁱⁱⁱ	162.26 (14)
O6—Te2—O8	91.15 (14)	Cu1 ⁱⁱⁱ —O4—Te1 ⁱⁱⁱ	55.74 (6)
O5—Te2—O8	71.82 (13)	Te2 ⁱ —O4—Te1 ⁱⁱⁱ	119.03 (9)
O4—Te2—O8	157.11 (13)	Te2—O4—Y1 ^{iv}	93.11 (12)
O3 ⁱⁱⁱ —Te2—O8	132.81 (11)	Cu1—O4—Y1 ^{iv}	87.45 (12)
O6—Te2—O2 ^{iv}	159.67 (12)	Y1 ^{ix} —O4—Y1 ^{iv}	72.00 (9)
O5—Te2—O2 ^{iv}	67.71 (13)	Cu1 ⁱⁱⁱ —O4—Y1 ^{iv}	176.66 (11)
O4—Te2—O2 ^{iv}	72.56 (12)	Te2 ⁱ —O4—Y1 ^{iv}	52.71 (5)
O3 ⁱⁱⁱ —Te2—O2 ^{iv}	111.52 (10)	Te1 ⁱⁱⁱ —O4—Y1 ^{iv}	122.87 (9)
O8—Te2—O2 ^{iv}	95.81 (12)	Te2—O5—Y1 ^x	136.03 (17)
O5 ^v —Y1—O2	154.82 (12)	Te2—O5—Y1 ^{ix}	99.64 (14)
O5 ^v —Y1—O1 ⁱ	111.21 (12)	Y1 ^x —O5—Y1 ^{ix}	108.37 (12)
O2—Y1—O1 ⁱ	80.12 (12)	Te2—O5—Te1 ^{iv}	100.31 (13)
O5 ^v —Y1—O4 ^{vi}	78.52 (12)	Y1 ^x —O5—Te1 ^{iv}	117.78 (13)
O2—Y1—O4 ^{vi}	112.44 (12)	Y1 ^{ix} —O5—Te1 ^{iv}	78.46 (10)
O1 ⁱ —Y1—O4 ^{vi}	129.31 (11)	Te2—O5—Cu1 ⁱⁱⁱ	64.46 (9)
O5 ^v —Y1—OW2	79.18 (12)	Y1 ^x —O5—Cu1 ⁱⁱⁱ	83.26 (10)
O2—Y1—OW2	83.29 (12)	Y1 ^{ix} —O5—Cu1 ⁱⁱⁱ	87.55 (9)
O1 ⁱ —Y1—OW2	72.67 (12)	Te1 ^{iv} —O5—Cu1 ⁱⁱⁱ	157.47 (12)
O4 ^{vi} —Y1—OW2	153.52 (12)	Te2—O6—Cu1 ⁱⁱⁱ	111.53 (16)
O5 ^v —Y1—OW1	84.04 (12)	Te2—O6—Te1 ⁱⁱⁱ	103.11 (14)
O2—Y1—OW1	78.45 (12)	Cu1 ⁱⁱⁱ —O6—Te1 ⁱⁱⁱ	86.06 (11)
O1 ⁱ —Y1—OW1	154.67 (12)	Te2—O6—Cu1	61.11 (9)
O4 ^{vi} —Y1—OW1	72.15 (12)	Cu1 ⁱⁱⁱ —O6—Cu1	69.15 (9)
OW2—Y1—OW1	91.49 (13)	Te1 ⁱⁱⁱ —O6—Cu1	58.27 (7)
O5 ^v —Y1—O5 ^{vi}	131.04 (10)	Te2—O6—Y1 ^x	78.26 (10)
O2—Y1—O5 ^{vi}	73.01 (11)	Cu1 ⁱⁱⁱ —O6—Y1 ^x	80.34 (10)
O1 ⁱ —Y1—O5 ^{vi}	73.74 (11)	Te1 ⁱⁱⁱ —O6—Y1 ^x	165.75 (11)
O4 ^{vi} —Y1—O5 ^{vi}	64.91 (11)	Cu1—O6—Y1 ^x	112.14 (9)
OW2—Y1—O5 ^{vi}	141.57 (12)	N1 ^{xi} —O7—Te1	111.3 (3)

OW1—Y1—O5 ^{vi}	112.16 (12)	N1 ^{xi} —O7—Te2 ⁱⁱ	149.8 (4)
O5 ^v —Y1—O2 ⁱ	72.04 (11)	Te1—O7—Te2 ⁱⁱ	66.47 (9)
O2—Y1—O2 ⁱ	132.19 (10)	N1 ^{xi} —O7—Y1	140.9 (4)
O1 ⁱ —Y1—O2 ⁱ	64.87 (11)	Te1—O7—Y1	67.08 (8)
O4 ^{vi} —Y1—O2 ⁱ	72.51 (11)	Te2 ⁱⁱ —O7—Y1	67.94 (6)
OW2—Y1—O2 ⁱ	113.51 (12)	N1—O8—Te2	111.0 (3)
OW1—Y1—O2 ⁱ	140.45 (11)	N1—O8—Te1 ^{iv}	123.8 (4)
O5 ^{vi} —Y1—O2 ⁱ	66.79 (12)	Te2—O8—Te1 ^{iv}	68.84 (9)
O1—Cu1—O4	179.67 (14)	N1—O8—Y1 ^x	163.7 (4)
O1—Cu1—O3 ⁱⁱⁱ	92.32 (14)	Te2—O8—Y1 ^x	71.18 (8)
O4—Cu1—O3 ⁱⁱⁱ	88.01 (14)	Te1 ^{iv} —O8—Y1 ^x	72.46 (7)
O1—Cu1—O6 ⁱ	87.95 (13)	N1 ^{xi} —O9—Te1	86.8 (3)
O4—Cu1—O6 ⁱ	91.72 (14)	N1 ^{xi} —O9—Te2 ^{xi}	81.0 (3)
O3 ⁱⁱⁱ —Cu1—O6 ⁱ	179.29 (14)	Te1—O9—Te2 ^{xi}	148.43 (17)
O1—Cu1—O1 ⁱⁱⁱ	95.24 (13)	N1 ^{xi} —O9—Te2 ⁱ	140.3 (3)
O4—Cu1—O1 ⁱⁱⁱ	84.92 (13)	Te1—O9—Te2 ⁱ	56.63 (6)
O3 ⁱⁱⁱ —Cu1—O1 ⁱⁱⁱ	68.03 (12)	Te2 ^{xi} —O9—Te2 ⁱ	138.25 (13)
O6 ⁱ —Cu1—O1 ⁱⁱⁱ	111.29 (12)	Y1—OW1—Te2 ⁱⁱ	96.11 (11)
O1—Cu1—O4 ⁱ	84.84 (13)	Y1—OW1—Cu1 ⁱⁱ	89.51 (11)
O4—Cu1—O4 ⁱ	94.99 (13)	Te2 ⁱⁱ —OW1—Cu1 ⁱⁱ	55.27 (6)
O3 ⁱⁱⁱ —Cu1—O4 ⁱ	112.68 (12)	Y1—OW1—Te2 ^v	77.63 (10)
O6 ⁱ —Cu1—O4 ⁱ	68.00 (12)	Te2 ⁱⁱ —OW1—Te2 ^v	165.76 (11)
O1 ⁱⁱⁱ —Cu1—O4 ⁱ	179.28 (9)	Cu1 ⁱⁱ —OW1—Te2 ^v	111.41 (9)
O9 ^{vii} —N1—O8	121.6 (5)	Y1—OW1—Cu1 ^{vi}	80.22 (9)
O9 ^{vii} —N1—O7 ^{vii}	120.0 (4)	Te2 ⁱⁱ —OW1—Cu1 ^{vi}	114.02 (10)
O8—N1—O7 ^{vii}	118.3 (5)	Cu1 ⁱⁱ —OW1—Cu1 ^{vi}	58.82 (6)
O9 ^{vii} —N1—Te2	77.9 (3)	Te2 ^v —OW1—Cu1 ^{vi}	52.63 (5)
O8—N1—Te2	48.7 (2)	Y1—OW1—H11	134 (5)
O7 ^{vii} —N1—Te2	151.4 (4)	Te2 ⁱⁱ —OW1—H11	83 (5)
O9 ^{vii} —N1—Te1 ^{vii}	71.9 (3)	Cu1 ⁱⁱ —OW1—H11	125 (5)
O8—N1—Te1 ^{vii}	165.1 (4)	Te2 ^v —OW1—H11	111 (5)
O7 ^{vii} —N1—Te1 ^{vii}	48.4 (2)	Cu1 ^{vi} —OW1—H11	142 (5)
Te2—N1—Te1 ^{vii}	138.27 (15)	Y1—OW1—H12	110 (5)
Cu1—O1—Te1	114.77 (16)	Te2 ⁱⁱ —OW1—H12	129 (5)
Cu1—O1—Y1 ⁱⁱⁱ	137.13 (17)	Cu1 ⁱⁱ —OW1—H12	82 (5)
Te1—O1—Y1 ⁱⁱⁱ	103.12 (14)	Te2 ^v —OW1—H12	45 (5)
Cu1—O1—Cu1 ⁱ	94.20 (13)	Cu1 ^{vi} —OW1—H12	37 (5)
Te1—O1—Cu1 ⁱ	83.41 (12)	H11—OW1—H12	106 (6)
Y1 ⁱⁱⁱ —O1—Cu1 ⁱ	109.90 (13)	Y1—OW2—Te1 ^{xii}	96.56 (11)
Cu1—O1—Te1 ⁱⁱⁱ	60.78 (9)	Y1—OW2—Cu1 ^{xii}	88.60 (11)
Te1—O1—Te1 ⁱⁱⁱ	143.74 (15)	Te1 ^{xii} —OW2—Cu1 ^{xii}	54.44 (6)
Y1 ⁱⁱⁱ —O1—Te1 ⁱⁱⁱ	76.93 (9)	Y1—OW2—Te1	77.77 (10)
Cu1 ⁱ —O1—Te1 ⁱⁱⁱ	131.38 (10)	Te1 ^{xii} —OW2—Te1	164.50 (12)
Cu1—O1—Te2 ⁱ	57.54 (9)	Cu1 ^{xii} —OW2—Te1	110.57 (10)
Te1—O1—Te2 ⁱ	68.88 (9)	Y1—OW2—Cu1 ⁱ	79.66 (10)
Y1 ⁱⁱⁱ —O1—Te2 ⁱ	163.46 (14)	Te1 ^{xii} —OW2—Cu1 ⁱ	112.61 (10)
Cu1 ⁱ —O1—Te2 ⁱ	55.85 (6)	Cu1 ^{xii} —OW2—Cu1 ⁱ	58.20 (6)
Te1 ⁱⁱⁱ —O1—Te2 ⁱ	118.32 (9)	Te1—OW2—Cu1 ⁱ	52.42 (5)

Cu1—O1—Y1 ^{viii}	87.20 (12)	Y1—OW2—H21	121 (5)
Te1—O1—Y1 ^{viii}	92.47 (11)	Te1 ^{xii} —OW2—H21	78 (5)
Y1 ⁱⁱⁱ —O1—Y1 ^{viii}	71.31 (9)	Cu1 ^{xii} —OW2—H21	128 (5)
Cu1 ⁱ —O1—Y1 ^{viii}	175.87 (11)	Te1—OW2—H21	117 (5)
Te1 ⁱⁱⁱ —O1—Y1 ^{viii}	52.60 (5)	Cu1 ⁱ —OW2—H21	157 (5)
Te2 ⁱ —O1—Y1 ^{viii}	122.26 (9)	Y1—OW2—H22	117 (5)
Te1—O2—Y1	136.04 (17)	Te1 ^{xii} —OW2—H22	128 (5)
Te1—O2—Y1 ⁱⁱⁱ	98.37 (14)	Cu1 ^{xii} —OW2—H22	86 (5)
Y1—O2—Y1 ⁱⁱⁱ	106.57 (12)	Te1—OW2—H22	47 (5)
Te1—O2—Te2 ⁱⁱ	101.48 (14)	Cu1 ⁱ —OW2—H22	46 (5)
Y1—O2—Te2 ⁱⁱ	118.61 (13)	H21—OW2—H22	112 (7)
Y1 ⁱⁱⁱ —O2—Te2 ⁱⁱ	77.90 (9)	Te1 ^{xiii} —OW3—Te2 ⁱⁱ	101.69 (12)
Te1—O2—Cu1 ⁱ	63.55 (9)	Te1 ^{xiii} —OW3—H31	77 (6)
Y1—O2—Cu1 ⁱ	82.11 (10)	Te2 ⁱⁱ —OW3—H31	59 (6)
Y1 ⁱⁱⁱ —O2—Cu1 ⁱ	86.71 (9)	Te1 ^{xiii} —OW3—H32	69 (6)
Te2 ⁱⁱ —O2—Cu1 ⁱ	156.91 (12)	Te2 ⁱⁱ —OW3—H32	66 (6)
Te1—O3—Cu1 ⁱ	112.24 (16)	H31—OW3—H32	106 (9)
Te1—O3—Te2 ⁱ	102.52 (15)		

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (ii) $x-1, -y+1/2, z-1/2$; (iii) $x, -y+1/2, z+1/2$; (iv) $x+1, -y+1/2, z+1/2$; (v) $x-1, -y+1/2, z-3/2$; (vi) $x-1, y, z-1$; (vii) $-x+1, y-1/2, -z+3/2$; (viii) $x, y, z+1$; (ix) $x+1, y, z+1$; (x) $x+1, -y+1/2, z+3/2$; (xi) $-x+1, y+1/2, -z+3/2$; (xii) $x, y, z-1$; (xiii) $-x, -y+1, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
OW1—H11 \cdots OW3	0.89 (3)	1.96 (3)	2.854 (6)	174 (7)
OW1—H12 \cdots O6 ^v	0.89 (3)	1.88 (4)	2.729 (5)	157 (7)
OW2—H21 \cdots O8 ^v	0.89 (3)	2.41 (6)	3.074 (5)	132 (6)
OW2—H21 \cdots OW3 ^{xiv}	0.89 (3)	2.22 (5)	2.949 (6)	139 (6)
OW2—H22 \cdots O3	0.89 (3)	1.95 (5)	2.745 (5)	149 (7)
OW3—H31 \cdots O7	0.90 (3)	1.97 (4)	2.834 (7)	162 (9)
OW3—H31 \cdots O8 ^{xi}	0.90 (3)	2.53 (8)	3.141 (7)	126 (7)
OW3—H32 \cdots O9 ^{xv}	0.89 (3)	2.49 (4)	3.360 (7)	166 (9)
OW3—H32 \cdots O9 ^{xiii}	0.89 (3)	2.64 (9)	3.253 (8)	127 (8)

Symmetry codes: (v) $x-1, -y+1/2, z-3/2$; (xi) $-x+1, y+1/2, -z+3/2$; (xiii) $-x, -y+1, -z+1$; (xiv) $-x, -y+1, -z$; (xv) $x-1, y, z$.