A new telluride topology: the crystal structure of honeaite Au$_3$TlTe$_2$

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ABSTRACT

The crystal structure of the first thallium-bearing gold telluride, honeaite Au$_3$TlTe$_2$, is reported and its topological novelty discussed. Honeaite is orthorhombic, space group *Pbcm* and unit-cell parameters $a = 8.9671(4)$, $b = 8.8758(4)$, $c = 7.8419(5)$ Å, $V = 624.14(6)$ Å^3 ($Z = 4$). Its structure has been refined to $R_1 = 0.033$, $wR_2 = 0.053$, Goof = 1.087. The structure is based upon a corrugated double-sheet comprising two sub-sheets, each composed of six-membered rings of corner-linked TeAu$_3$ pyramids in which the Te lone pair is stereoactive. Rows of thallium atoms lie in the grooves between sheets and provide the only inter-sheet connectivity *via* Tl-Au bonds. There is extensive Au-Au bonding linking the two sub-sheets of the double-sheet. The structure is distinct from those of the 1:2 (Au,Ag)-tellurides: calaverite AuTe$_2$, sylvanite AuAgTe$_4$ and krennerite Au$_3$AgTe$_8$, which are based upon sheet structures with no connecting inter-sheet atoms. It also differs fundamentally from the structures of synthetic phases Ag$_3$TlTe$_2$ and Ag$_{18}$Tl$_4$Te$_{11}$, both of which have an analogous stoichiometry. In contrast to the pyramidal TeAu$_3$ group of honeaite and krennerite, Ag does not form the corresponding TeAg$_3$ group in its tellurides.

Introduction

TELLURIUM is one of the few elements to form stoichiometric compounds with gold in nature. Recently, a new natural gold telluride was found at the Karonie gold deposit in the Eastern Goldfields region of the Yilgarn Craton, Western Australia. The telluride has a novel composition Au$_3$TlTe$_2$ and structure. There is no synthetic analogue. The mineral is named honeaite after the mineralogist Russell M. Honea (1929–2002) who, amongst many diverse achievements in geology, published the original description of the geology and mineralogy of the Karonie deposit. The mineral and name have been approved by the International Mineralogical Association as a new species (Rice *et al.*, 2015). The geological occurrence, petrogenesis and formal mineralogical description of honeaite are described in a separate paper (Rice *et al.*, 2016).

It appears that a honeaite-like natural phase was found by Nechaev and Cook (2000) at the Maiskoe gold deposit in Ukraine. Two microprobe analyses were reported that gave compositions (Te = 2 atoms per formula unit) of Au$_{3.38}$Tl$_{1.14}$Te$_2$Sb$_{0.03}$ and Au$_{3.22}$Ag$_{0.02}$Tl$_{1.00}$Te$_2$Sb$_{0.03}$. No crystal structure or unit-cell parameters were reported and no new-mineral description was submitted to the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association or a name chosen. Consequently, while the composition is essentially that of honeaite, it is unclear if it is actually this mineral. It would be of interest to obtain a suitable sample of this material for structure determination to see if it is indeed honeaite. Here, we report the determination of the structure of honeaite and discuss its topological significance and distinctiveness.

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Sample material

The crystal used in the structure determination reported below came from a rock core sample collected at the Archaean Karonie gold deposit of the Eastern Goldfields province of Western Australia. The geological occurrence of the new mineral honeaite is reported by Rice *et al*. (2016). The type specimen and crystal are held in the collection of the Natural History Museum (London) under catalogue number BM2015,36.

Chemical analyses of 17 grains of honeaite (one analysis per grain) in a polished thin section were obtained, including for the type crystal, by electron microprobe analysis using energy dispersive spectrometry (EDS) operated at 15 kV, 2.8 nA, with a beam diameter of ~0.005 mm and a live-time of 200 s. The element standards used were: Au metal (Au), thallium iodide (Tl) and Te metal (Te). No other elements were detected in EDS survey scans. Analytical totals were 99.60–101.02%. The average composition of 17 analyses is 56.33(0.37) wt.% Au, 19.68(0.27) wt.% Tl and 24.30(0.11) wt.% Te. The corresponding average chemical formula is $Au_{2.996}Tl_{1.009}Te_{1.995}$. A spot analysis of the type crystal gave 56.19 wt.% Au, 19.45 wt.% Tl and 24.19 wt.% Te, with a corresponding chemical formula of $Au_{3.003}Tl_{1.002}Te_{1.996}$.

X-ray diffraction

Experimental methods and materials

A polished petrographic thin section (0.03 mm thick) was surveyed by electron microprobe analysis and numerous crystals of the new phase were identified as having a distinctive new composition close to Au_3TlTe_2. A small rectangular, flake-like crystal (0.040 mm × 0.035 mm × 0.015 mm) was extracted from the thin section by excavating with a fine acupuncture needle (0.008 mm tip) and attached to a non-diffracting amorphous carbon fibre (0.01 mm diameter) itself glued to a glass fibre support. Data were collected using an XcaliburE single-crystal X-ray diffractometer equipped with an EoS CCD detector (®Rigaku Oxford Diffraction) and graphite-monochromatized Mo*Kα* radiation operated at 45 kV, 40 mA. The data collection strategy used was chosen on the basis of a 2-hour pre-experiment. A whole sphere of reflections was collected to 60°2θ. Information relating to the data collection is given in Table 1. Raw reflection intensities were corrected for Lorentz and polarization effects and for absorption, the latter by the

TABLE 1. Summary of the data collection and structure refinement of honeaite.

Crystal data	
Ideal chemical formula	Au_3TlTe_2
Space group	*Pbcm*
a (Å)	8.9671(4)
b (Å)	8.8758(4)
c (Å)	7.8419(5)
V (Å^3)	624.14(6)
Z	4
Dx (Mg m^{-3}) calc	11.18
μ (mm^{-1})	105.05
Data collection	
Diffractometer	Xcalibur E (1 K Eos detector)
Radiation, wavelength (Å)	Mo*Kα*, 0.71073
Crystal	Opaque rectangular plate
Max. Med. Min. dimensions (mm)	0.040 × 0.035 × 0.015
Temperature (K)	293(2)
Scan type, frame-width (°), frame-time (s)	ω, 1.0, 240
Absorption correction	Multi-scan
T_{min}, T_{max}	0.233, 1
Refl. used for cell, $I > 7\sigma(I)$	1903
Refl. measured	11,673
R_σ	0.030
Independent refl.	1136
Independent refl. with $I > 2\sigma(I)$	948
R_{int} (*mmm*)	0.058
θ$_{min}$, θ$_{max}$ (°)	3.22, 31.91
Index range	$-12 \leq h \leq 13$, $-12 \leq k \leq 13$, $-11 \leq l \leq 11$
Data completeness to 30°θ (%)	99.9
Refinement	
Refl., restraints, parameters	1136, 0, 34
$R_1[I > 2\sigma(I)]$, R_1(all)	0.033, 0.046
$wR_2[I > 2\sigma(I)]$, wR_2(all)	0.050, 0.053
Goof (F^2)	1.087
Weighting scheme*	$a = 0.0178$
$(\Delta/\sigma)_{max}$	<0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (*e* Å^{-3})	2.1, −3.6

* SHELX (Sheldrick, 2008)

multi-scan method (averaging of equivalent reflections) in the program *CrysalisPro* (®Rigaku Oxford Diffraction) and converted to structure factors.

Results

Structure refinement

The unit-cell of honeaite is metrically orthorhombic and systematic absences indicated space group

Pbcm. The structure was solved by Direct Methods and refined using *SHELX* (Sheldrick, 2008). Neutral atomic scattering factors taken from *International Tables for Crystallography* (Wilson, 1992) were used. Information relating to the data collection and structure refinement is summarized in Table 1. Atom coordinates and displacement parameters are given in Table 2; key interatomic distances are given in Table 3. A crystallographic information file has been deposited with the Principal Editor of *Mineralogical Magazine* and is available from http://www.minersoc.org/pages/e_journals/dep_mat_mm.html

The structure was solved and refined using *SHELX* (Sheldrick, 2008) within the *WinGX* program suite (Farrugia, 1999). All six atoms of the asymmetric unit were found by structure solution using direct methods. There are two Te, three Au and one Tl in the asymmetric unit; all atoms have site multiplicity 4. Assignment of Te *vs*. (Au, Tl) used site scattering values (50 *vs*. 79/81 electrons). Assignment of Au ($Z = 79$) *vs*. Tl ($Z = 81$) was based upon crystal chemical reasoning: observed Te bond distances, all of which are almost identical (2.607−2.620 Å) and topological similarity with Te coordination in calaverite, $AuTe_2$, strongly point to the presence of $TeAu_3$ groups. A Te–Au distance of 2.61 Å occurs in calaverite (Schütte and de Boer, 1988). The highly regular nature of the $TeAu_3$ group (bonds and angles) indicates that a single type of element coordinates Te in this group, i.e. Au. It cannot be $TeTl_3$ because this would require a much higher Tl content than the empirical formula has. Mixed $Te(Tl,Au)_3$ is unsupported by the bond lengths, all of which are almost the same and recognizable as Te-Au distances in related minerals calaverite, sylvanite and krennerite (Schütte and de Boer, 1988; Tunell, 1941; Dye and Smyth, 2012). Finally, Au−Au distances are 2.87−2.91 Å and are very similar to that of elemental gold (2.87 Å). Consequently, we assign all Au to the sites at 2.61 Å from Te and forming $TeAu_3$ groups. The maximum residual unmodelled electron density of 2 $e/Å^3$ lies at 2.06 Å from Te(2) and is unassigned.

Structure topology

The structural features of honeaite are shown Figs. 1–4. The structure comprises corrugated sheets of connected 6-membered rings of $TeAu_3$ groups ||(100) as shown in Figs 1 and 2. Individual sheets comprise alternating chains of $Te(1)Au_3$ and $Te(2)Au_3$ pyramids. The overall structure is

TABLE 2. Atom coordinates and displacement parameters U^{ij} (Å^2) for honeaite.

Atom	x/a	y/b	z/c	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	U_{eq}
Tl	0.21609(5)	¾	0	0.0196(3)	0.0263(3)	0.0255(3)	0.0043(2)	0	0	0.0238(1)
Au(1)	-0.13342(5)	¾	0	0.0173(2)	0.0177(2)	0.0155(3)	0.0004(2)	0	0	0.0168(1)
Au(2)	0.54678(5)	¾	0	0.0169(2)	0.0247(3)	0.0205(3)	-0.0064(2)	0	0	0.0207(1)
Au(3)	0.17523(5)	0.48884(5)	¼	0.0156(2)	0.0161(2)	0.0186(3)	0	0	0.0018(2)	0.0167(1)
Te(1)	0.10918(9)	0.05618(8)	¼	0.0143(4)	0.0152(4)	0.0150(4)	0	0	-0.0002(3)	0.0148(2)
Te(2)	0.53752(8)	0.55678(8)	−¼	0.0150(4)	0.0145(4)	0.0154(5)	0	0	0.0003(3)	0.0150(2)

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TABLE 3. Interatomic distances in honeaite (Å).

Au(1)		Tl	
Te(1) × 2	2.6173(5)	Au(2)	2.9653(7)
Au(2)	2.8677(7)	Au(3) ×2	3.0579(4)
Au(3) ×2	2.9117(3)	Au(1)	3.1341(7)
Tl	3.1341(7)	Te(1) ×2	3.4854(7)
Au(2)		Te(1)	
Te(2) × 2	2.6061(5)	Au(1) ×2	2.6173(5)
Au(1)	2.8677(7)	Au(3)	2.620(1)
Tl	2.9653(7)		
Au(3)		Te(2)	
Te(2)	2.6074(9)	Au(2) ×2	2.6061(5)
Te(1)	2.620(1)	Au(3)	2.6074(9)
Au(1) ×2	2.9117(3)		
Tl ×2	3.0579(4)		

composed of stacked double-sheets in which Au–Au bonds connect the two sub-sheets (Fig. 2). Adjacent double-sheets are connected *via* Tl–Au(2) bonds (2.966 Å). Rows of thallium atoms extend ‖ [001] and lie in the grooves between sheet corrugations.
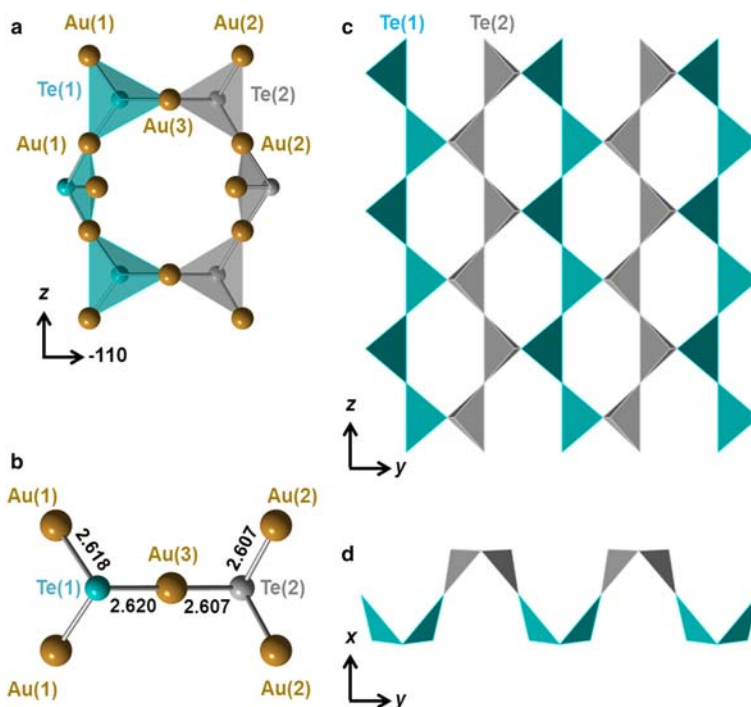

FIG. 1. (*a*) The six-membered ring comprising fused chains of Te(1)Au$_3$ and Te(2)Au$_3$ pyramids. (*b*) A pair of Te(1)Au$_3$ and Te(2)Au$_3$ pyramids with Te–Au bond lengths shown. The apex (Te) of the Te(1)Au$_3$ pyramid points up, that of the Te (2)Au$_3$ pyramid points down. (*c*) Connected six-membered rings forming a corrugated sheet composed of alternating rows of Te(1)Au$_3$ and Te(2)Au$_3$ pyramids. (*d*) The same sheet as in (*c*) projected onto (001) and showing the nature of the sheet corrugation.
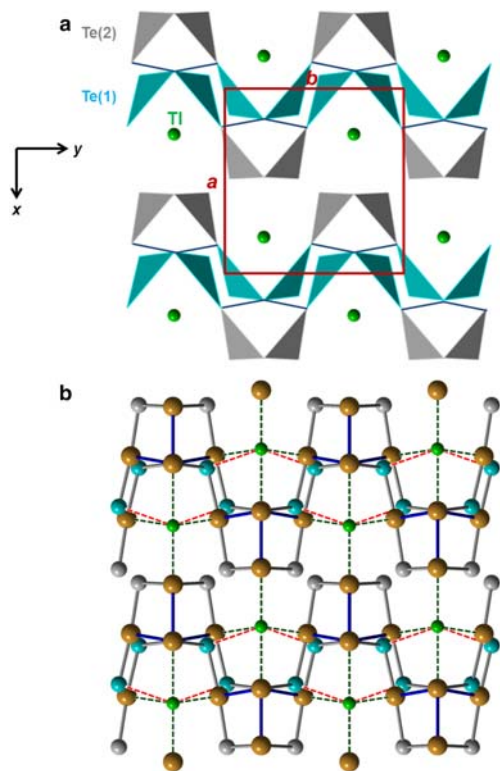
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FIG. 2. (*a*) Polyhedral representation of the honeaite structure showing corrugated layers composed of double-sheets of TeAu$_3$ pyramids with rows of thallium atoms (green spheres) occupying grooves in sheet corrugations extending parallel to [001]. (*b*) A ball-and-spoke representation of (*a*) showing Tl–Au bonds (dashed black lines), Tl···Te distances (dashed red lines) and intra-sheet Au–Au bonds (solid blue lines).

Thallium is coordinated to four Au atoms with bond lengths of 2.96–3.13 Å. There are also two very long distances to Te(1) atoms (3.49 Å), leading to an octahedral environment (Fig. 3). The exact nature of the Tl−Te distance is unclear, as the role of the Te lone pair is undefined. The thallium site is very different from the three Au sites.

TeAu$_3$ groups

All Te and Au atoms form TeAu$_3$ groups in which Te is displaced to one side of the triangle of Au atoms and is characteristic of lone-pair stereo-activity. The two non-equivalent TeAu$_3$ groups are highly regular flattened triangular-based pyramids

with Te–Au distances of 2.607−2.620 Å and Au–Te–Au angles of 97–103°. The polyhedral environments of Te(1)Au$_3$ and Te(2)Au$_3$ are very different, as illustrated in Fig. 4. The Te(1)Au$_3$ pyramid shares two edges with TlAu$_4$ groups and apices with two Te(1)Au$_3$ and one Te(2)Au$_3$. The Te(2)Au$_3$ pyramid has no shared edges, but is corner-linked to two Te(2)Au$_3$, one Te(1)Au$_3$ and two TlAu$_4$.

Au polyhedra

The three Au sites (Fig. 3) have different coordination environments. The Au(1) and Au(3) sites are octahedrally-coordinated, whereas Au(2) is four-fold coordinated. The Au(1) site is bonded to two Te, three Au atoms and one Tl atom; Au(3) is bonded to two Te, two Au and two Tl atoms; Au(2) is bonded to two Te atoms, one Au atom and one Tl atom. The Au−Au distances are 2.87–2.91 Å and are very similar to that of elemental gold (2.87 Å). The Au–Tl bonds are 2.97–3.06 Å and the Te–Au bonds are all very similar at 2.61–2.62 Å. The connectivity of the Au polyhedra is shown in Fig. 3. The two octahedra (Au 1,3) share an edge and the four-coordinate Au(2) quadrilateral interpenetrates the Au(1) octahedron.

Thallium

As described above, the assignment of Tl *vs.* Au sites can be made using crystal chemical reasoning. The four nearly coplanar Tl–Au bonds are long (2.97–3.13 Å) and uncharacteristic of Au–Au, one of which, Tl–Au(2), links adjacent double-sheets. Two very long distances (3.49 Å) to Te(1) atoms suggest octahedral coordination of Tl, although it is questionable if these two distances are meaningful bonds. The TlAu$_4$ groups are corner-connected to form rows ∥[001].

Discussion

The synthetic compounds CsAu$_3$S$_2$, RbAu$_3$Se$_2$ and CsAu$_3$Se$_2$ (Klepp and Weithaler, 1996) have an analogous stoichiometry to that of honeaite, but the monovalent species is an alkali metal, whereas it is thallium in honeaite. The structure topology shared by these three compounds comprises alternating planar sheets of SeAu$_3$ (SAu$_3$) pyramids and Cs (Rb) atoms, and contrasts with the corrugated sheet of honeaite. Furthermore, the coordination of Se and S atoms is very different from Te in honeaite: Se and S are octahedrally-coordinated to three Au
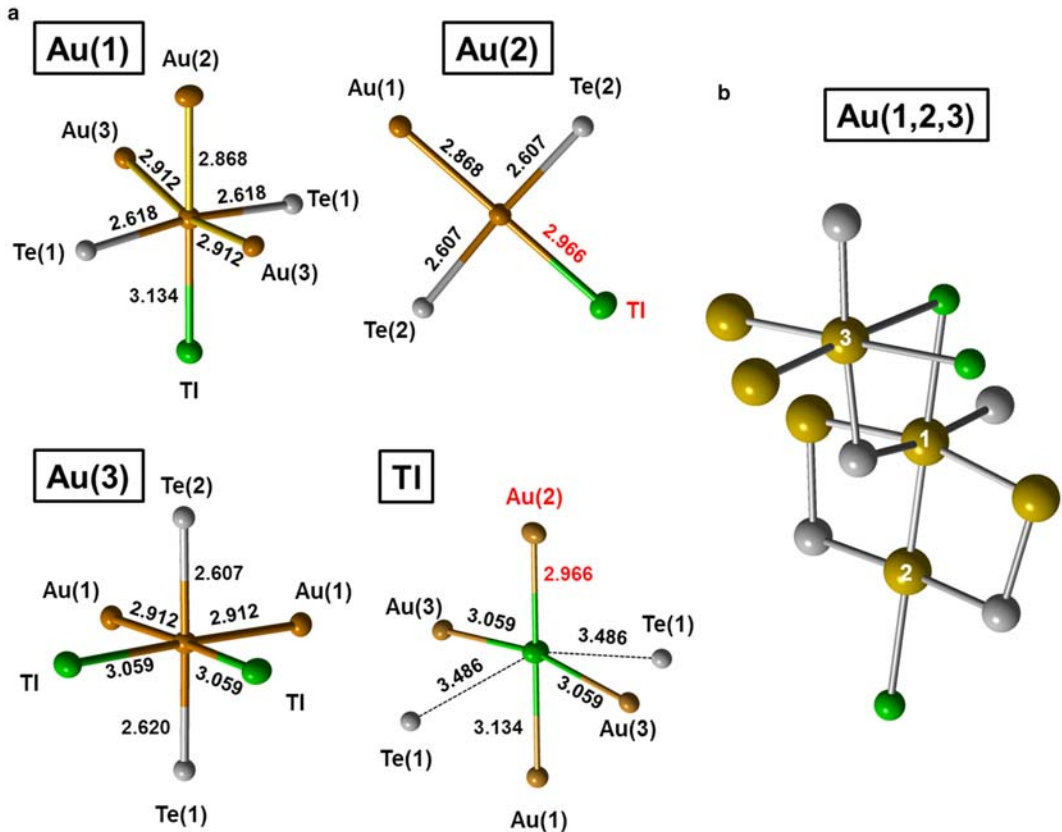
Fig. 3. (*a*) Coordination and bond distances (Å) of Au and Tl atoms in honeaite. Au(1) and Au(3) form octahedra, whereas Au(2) is four-coordinate, including an inter-sheet Au–Tl bond (highlighted in red). Tl–Te distances are shown as dotted black lines and may not correspond to real bonds. Anisotropic displacement parameters are drawn at the 68% level. (*b*) Polyhedral connectivity of the three Au sites of honeaite. All atoms are drawn as spheres and central Au sites are numbered.

and three Cs (Rb) cations, e.g. $Se[Au_3Cs_3]$ in $CsAu_3Se_2$.

One of the two non-equivalent Te atoms of honeaite has possible bonding distances to Tl, whereas the other Te is only bonded to Au. In both cases, $Te[Au_3Tl_2]$ and $Te[Au_3]$, the coordination is highly asymmetric (one-sided), suggesting stereo-activity of both Te atoms. For $CsAu_3Se_2$ and $CsAu_3S_2$, the Cs–Se and Cs–S distances of 3.76 and 3.73 Å, respectively, imply that the Te(1)–Tl distance at 3.49 Å in honeaite is likely to be a bond, albeit contributing little bond valence to Te. Much longer Te–Tl distances in honeaite (>3.9 Å) are very unlikely to be bonds and if included would result in very unusual coordination for Te. Thus, Tl can be considered to be octahedrally-coordinated. This coordination environment is very different

from that of Cs and Rb in $CsAu_3S_2$, $RbAu_3Se_2$ and $CsAu_3Se_2$, in which they are octahedrally-coordinated by six Se (S) atoms.

Three gold telluride minerals related to honeaite are calaverite $AuTe_2$, sylvanite $AuAgTe_4$ and krennerite Au_3AgTe_8 (Dye and Smyth, 2012), all of which have general 1:2 stoichiometry (Au, Ag) Te_2. Honeaite is the only gold telluride with essential thallium. While calaverite, krennerite and honeaite have very different topologies, they share some features, such as $TeAu_3$ pyramids and octahedrally-coordinated Au. However, krennerite has $TeAu_3$ pyramids that are much more distorted than those of honeaite. The 1:2 compounds have a sheet of edge-sharing $(Au,Ag)Te_6$ octahedra; in sylvite and krennerite there are alternating rows of $AuTe_6$ and $AgTe_6$. In calaverite and sylvanite these

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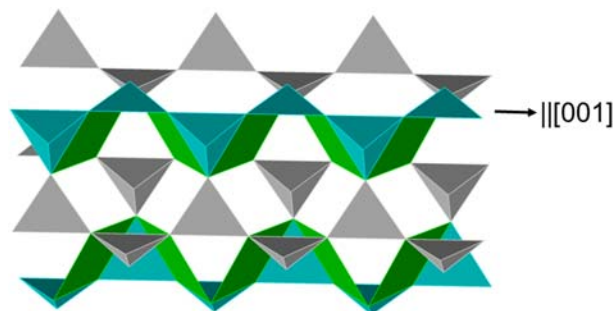
FIG. 4. Fragment of the honeaite structure viewed slightly obliquely to the *y* axis and showing the very different polyhedral connectivities of Te(1)Au$_3$ (blue) and Te(2)Au$_3$ (grey) pyramids. Chains of TeAu$_3$ pyramids of the corrugated sheets extend parallel to [001]. For each pyramid the Te atom is located at the apex that is not bonded to other polyhedra. TlAu$_4$ groups are shown green and each shares two edges with Te(1)Au$_3$ pyramids.

sheets are planar with dative bonding involving Te providing the only inter-sheet connectivity. In krennerite the sheets are folded in a zigzag arrangement; again dative bonding involving Te is the only inter-sheet connection. In contrast to these 1:2 sheet structures, honeaite does not appear to have dative bonding; the only linkages between double-sheets are Tl-Au bonds.

It has been suggested that the short Te···Te distance of 2.84 Å in krennerite Au$_3$AgTe$_8$ may be associated with Te···Te inter-sheet bonding (Dye and Smyth, 2012). Indeed, no other options appear to be possible for bonding between the sheets. Sylvanite AgAuTe$_4$, another sheet structure, has a Te···Te inter-sheet distance of 2.89 Å. Calaverite AuTe$_2$, has a shortest inter-sheet Te···Te distance of 3.20 Å. The shortest inter-sheet Te···Te and Te-Au distances in honeaite are 4 Å, and as such are likely to be far too long to correspond to dative bonds. Hence, the only significant inter-sheet bonding in honeaite is *via* the Tl-Au(2) bond (2.97 Å).

There are two synthetic silver-thallium-tellurides having an analogous Ag$_3$TlTe$_2$ stoichiometry: Ag$_3$TlTe$_2$ Cenzual *et al.* (1991) and Ag$_{18}$Tl$_4$Te$_{11}$ (Brun *et al.*, 1992). Both have very different structures from each other and from that of honeaite. Ag$_3$TlTe$_2$ (orthorhombic, *Cmmm*) is an Ag-Te framework with strong compositional layering and Tl in [8]-coordination Tl(Ag$_4$Te$_4$). Whereas Ag$_{18}$Tl$_4$Te$_{11}$ (cubic, *F$\bar{4}$3m*) is an Ag-Te framework with channels occupied by Tl$_6$ octahedral clusters. In both compounds Te has high coordination ≥[6].

Finally, petzite Ag$_3$AuTe$_2$ (Haidinger 1845 cited by Frueh, 1959) and fischesserite Ag$_3$AuSe$_2$ (Bindi and Cipriani, 2004) have the same 3:1:2 stoichiometry but very different structures from that of honeaite.

Honeaite is a new gold telluride structure. The Tl site has four bonds to Au at ~3 Å and two long Tl–Te bonds. It may be possible for Au or Ag to occupy a similar, albeit more contracted, site. The possibility may, therefore, exist of a new class of 2:1 gold tellurides (Au,Ag)$_2$Te based upon the honeaite topology. We are not aware of any synthetic Au–Tl–Te phases, and so the wider significance of Tl for structural diversity in gold tellurides remains to be explored.

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