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1 **REVISION 1**

2 **A new telluride topology: the crystal structure of honeaite Au₃TlTe₂.**

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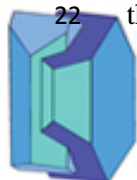
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9 Key words: honeaite, new mineral, crystal structure, telluride

10 **Abstract**

11 The crystal structure of the first thallium-bearing gold telluride, honeaite Au₃TlTe₂, is
12 reported and its topological novelty discussed. Honeaite is orthorhombic, space group *Pbcm*
13 and unit-cell parameters $a = 8.9671(4) \text{ \AA}$, $b = 8.8758(4) \text{ \AA}$, $c = 7.8419(5) \text{ \AA}$, $V = 624.14(6)$
14 \AA^3 ($Z = 4$). Its structure has been refined to $R_1 = 0.033$, $wR_2 = 0.053$, $GoF = 1.087$. The
15 structure is based upon a corrugated double-sheet comprising two sub-sheets, each composed
16 of six-membered rings of corner-linked TeAu₃ pyramids in which the Te lone-pair is
17 stereoactive. Rows of thallium atoms lie in the grooves between sheets and provide the only
18 inter-sheet connectivity *via* Tl-Au bonds. There is extensive Au-Au bonding linking the two
19 sub-sheets of the double-sheet. The structure is distinct from those of the 1:2 (Au,Ag)-
20 tellurides calaverite AuTe₂, sylvanite AuAgTe₄, and krennerite Au₃AgTe₈, which are based
21 upon sheet structures with no connecting inter-sheet atoms. It also differs fundamentally from
22 the structures of synthetic phases Ag₃TlTe₂ and Ag₁₈Tl₄Te₁₁, both of which have an



23 analogous stoichiometry. In contrast to the pyramidal TeAu_3 group of honeaite and
24 krennerite, Ag does not form the corresponding TeAg_3 group in its tellurides.

25

26 **Introduction**

27 Tellurium is one of the few elements to form stoichiometric compounds with gold in
28 nature. Recently, a new natural gold telluride was found at the Karonie gold deposit in the
29 Eastern Goldfields region of the Yilgarn Craton, Western Australia. The telluride has a novel
30 composition Au_3TlTe_2 and structure. There is no synthetic analogue. The mineral is named
31 honeaite after the mineralogist Russell M. Honea (1929-2002) who, amongst many diverse
32 achievements in geology, published the original description of the geology and mineralogy of
33 the Karonie deposit. The mineral and name have been approved by the International
34 Mineralogical Association as a new species (Rice et al. 2015). The geological occurrence,
35 petrogenesis and formal mineralogical description of honeaite are described in a separate
36 paper (Rice et al. in press).

37 It appears that a honeaite-like natural phase was found by Nechaev and Cook (2000)
38 at the Maiskoe gold deposit in Ukraine. Two microprobe analyses were reported that gave
39 compositions ($\text{Te} = 2 \text{ apfu}$) of $\text{Au}_{3.38}\text{Tl}_{1.14}\text{Te}_2\text{Sb}_{0.03}$ and $\text{Au}_{3.22}\text{Ag}_{0.02}\text{Tl}_{1.00}\text{Te}_2\text{Sb}_{0.03}$. No crystal
40 structure or unit-cell parameters were reported and no formal new-mineral description was
41 submitted to IMA or a name chosen. Consequently, while the composition is essentially that
42 of honeaite, it is unclear if it is actually this mineral. It would be of interest to obtain a
43 suitable sample of this material for structure determination to see if it is indeed honeaite.
44 Here, we report the determination of the structure of honeaite and discuss its topological
45 significance and distinctiveness.

46

47 **Sample material**

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

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

63

64 **X-ray diffraction**

65 *Experimental methods and materials*

66 A polished petrographic thin section (0.03 mm thick) was surveyed by electron
67 microprobe analysis and numerous crystals of the new phase were identified as having a
68 distinctive new composition close to Au_3TlTe_2 . A small rectangular, flake-like crystal (0.040

69 $\times 0.035 \times 0.015$ mm) was extracted from the thin section by excavating with a fine
70 acupuncture needle (0.008 mm tip) and attached to a non-diffracting amorphous carbon fibre
71 (0.01 mm diameter) itself glued to a glass fibre support. Data were collected using an
72 XcaliburE single-crystal X-ray diffractometer equipped with an EoS CCD detector ([®]Rigaku
73 Oxford Diffraction) and graphite-monochromatised MoK α radiation operated at 45 kV, 40
74 mA. The data collection strategy used was chosen on the basis of a 2-hour pre-experiment. A
75 whole sphere of reflections was collected to 60° 2 θ . Information relating to the data collection
76 is given in **Table 1**. Raw reflection intensities were corrected for Lorentz and polarisation
77 effects and for absorption, the latter by the multi-scan method (averaging of equivalent
78 reflections) in the program *CrysalisPro* ([®]Rigaku Oxford Diffraction) and converted to
79 structure factors.

80

81 **Results**

82 *Structure refinement*

83 The unit-cell of honeaite is metrically orthorhombic and systematic absences
84 indicated space group *Pbcm*. The structure was solved by Direct Methods and refined using
85 SHELX (Sheldrick, 2008). Neutral atomic scattering factors taken from *International Tables*
86 *for Crystallography* (Wilson, 1992) were used. Information relating to the data collection and
87 structure refinement is summarised in **Table 1**. Atom coordinates and displacement
88 parameters are given in **Table 2**; key interatomic distances are given in **Table 3**. A CIF file is
89 deposited with the journal.

90 The structure was solved and refined using SHELX (Sheldrick, 2008) within the
91 WinGX program suite (Farrugia, 1999). All six atoms of the asymmetric unit were found by

92 structure solution using Direct Methods. There are two Te, three Au and one Tl in the
93 asymmetric unit; all atoms have site multiplicity 4. Assignment of Te versus (Au, Tl) used
94 site scattering values (50 versus 79/81 electrons). Assignment of Au ($Z = 79$) versus Tl ($Z =$
95 81) was based upon crystal chemical reasoning: observed Te bond distances, all of which are
96 almost identical ($2.607\text{--}2.620 \text{ \AA}$) and topological similarity with Te coordination in
97 calaverite, AuTe_2 , strongly point to the presence of TeAu_3 groups. A Te-Au distance of 2.61
98 \AA occurs in calaverite (Schütte and de Boer, 1988). The highly regular nature of the TeAu_3
99 group (bonds and angles) indicates that a single type of element coordinates Te in this group,
100 i.e. Au. It cannot be TeTl_3 because this would require a much higher Tl content than the
101 empirical formula has. Mixed Te(Tl,Au)_3 is unsupported by the bond lengths, all of which are
102 almost the same and recognisable as Te-Au distances in related minerals calaverite, sylvanite
103 and krennerite (Schütte and de Boer, 1988; Tunell, 1941; Dye and Smyth, 2012). Finally,
104 Au–Au distances are $2.87\text{--}2.91 \text{ \AA}$ and are very similar to that of elemental gold (2.87 \AA).
105 Consequently, we assign all Au to the sites at 2.61 \AA from Te and forming TeAu_3 groups.
106 The maximum residual unmodelled electron density of 2 e/\AA^3 lies at 2.06 \AA from Te(2) and is
107 unassigned.

108

109 **Structure topology**

110 The structural features of honeaitite are shown **Figures 1-4**. The structure comprises
111 corrugated sheets of connected 6-membered rings of TeAu_3 groups $\parallel(100)$ as shown in
112 **Figures 1 and 2**. Individual sheets comprise alternating chains of Te(1)Au_3 and Te(2)Au_3
113 pyramids. The overall structure is composed of stacked double-sheets in which Au-Au bonds
114 connect the two sub-sheets (**Fig. 2**). Adjacent double-sheets are connected only *via* Tl-Au

115 bonds (2.966 Å). Rows of thallium atoms extend ||[001] and lie in the grooves between sheet
116 corrugations.

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

121 *TeAu₃ groups*

122 All Te and Au atoms form TeAu₃ groups in which Te is displaced to one side of the
123 triangle of Au atoms and is characteristic of lone-pair stereoactivity. The two non-equivalent
124 TeAu₃ groups are highly regular flattened triangular-based pyramids with Te–Au distances of
125 2.607–2.620 Å and Au–Te–Au angles of 97–103°. The polyhedral environments of Te(1)Au₃
126 and Te(2)Au₃ are very different, as illustrated in **Figure 4**. The Te(1)Au₃ pyramid shares two
127 edges with TlAu₄ groups and apices with two Te(1)Au₃ and one Te(2)Au₃. The Te(2)Au₃
128 pyramid has no shared edges, but is corner-linked to two Te(2)Au₃, one Te(1)Au₃ and two
129 TlAu₄.

130

131 *Au polyhedra*

132 The three Au sites (**Fig. 3**) have different coordination environments. Au(1) and
133 Au(3) are octahedrally-coordinated, whereas Au(2) is four-fold coordinated. Au(1) is bonded
134 to two Te, three Au atoms and one Tl atom; Au(3) is bonded to two Te, two Au and two Tl
135 atoms; Au(2) is bonded to two Te atoms, one Au atom and one Tl atom. Au–Au distances are
136 2.87 – 2.91 Å and are very similar to that of elemental gold (2.87 Å). Au–Tl bonds are 2.97 –
137 3.06 Å. Te–Au bonds are all very similar at 2.61 – 2.62 Å. The connectivity of the Au

138 polyhedra is shown in **Figure 3**. The two octahedra (Au 1,3) share an edge and the four-
139 coordinate Au(2) quadrilateral interpenetrates the Au(1) octahedron.

140

141 *Thallium*

142 As described above, the assignment of Tl *versus* Au sites can be made using crystal
143 chemical reasoning. The four nearly coplanar Tl-Au bonds are long (2.97 – 3.13 Å) and
144 uncharacteristic of Au-Au, one of which, Tl-Au(2), links adjacent double-sheets. Two very
145 long distances (3.49 Å) to Te(1) atoms suggest octahedral coordination of Tl, although it is
146 questionable if these two distances are meaningful bonds. TlAu₄ groups are corner-connected
147 to form rows ||[001].

148

149 **Discussion**

150 The synthetic compounds CsAu₃S₂, RbAu₃Se₂ and CsAu₃Se₂ (Klepp and Weithaler,
151 1996) have an analogous stoichiometry to that of honeaite, but the monovalent species is an
152 alkali metal, whereas it is thallium in honeaite. The structure topology shared by these three
153 compounds comprises alternating planar sheets of SeAu₃ (SAu₃) pyramids and Cs (Rb)
154 atoms, and contrasts with the corrugated sheet of honeaite. Furthermore, the coordination of
155 Se and S atoms is very different from Te in honeaite: Se and S are octahedrally-coordinated
156 to three Au and three Cs (Rb) cations, e.g. Se[Au₃Cs₃] in CsAu₃Se₂.

157 One of the two non-equivalent Te atoms of honeaite has possible bonding distances to
158 Tl, whereas the other Te is only bonded to Au. In both cases, Te[Au₃Tl₂] and Te[Au₃], the
159 coordination is highly asymmetric (one-sided), suggesting stereoactivity of both Te atoms.
160 For CsAu₃Se₂ and CsAu₃S₂, the Cs-Se and Cs-S distances of 3.76 and 3.73 Å, respectively,

161 imply that the Te(1)-Tl distance at 3.49 Å in honeaite is likely to be a bond, albeit
162 contributing little bond valence to Te. Much longer Te-Tl distances in honeaite (> 3.9 Å) are
163 very unlikely to be bonds and if included would result in very unusual coordination for Te.
164 Thus, Tl can be considered to be octahedrally-coordinated. This coordination environment is
165 very different from that of Cs and Rb in CsAu₃S₂, RbAu₃Se₂ and CsAu₃Se₂, in which they are
166 octahedrally-coordinated by six Se (S) atoms.

167 Three gold telluride minerals related to honeaite are calaverite AuTe₂, sylvanite
168 AuAgTe₄ and krennerite Au₃AgTe₈ (Dye and Smyth, 2012), all of which have general 1:2
169 stoichiometry (Au, Ag)Te₂. Honeaite is the only gold telluride with essential thallium. While
170 calaverite, krennerite and honeaite have very different topologies, they share some features,
171 such as TeAu₃ pyramids and octahedrally-coordinated Au. However, krennerite has TeAu₃
172 pyramids that are much more distorted than those of honeaite. The 1:2 compounds have a
173 sheet of edge-sharing (Au,Ag)Te₆ octahedra; in sylvite and krennerite there are alternating
174 rows of AuTe₆ and AgTe₆. In calaverite and sylvanite these sheets are planar with dative
175 bonding involving Te providing the only inter-sheet connectivity. In krennerite the sheets are
176 folded in a zigzag arrangement; again dative bonding involving Te is the only inter-sheet
177 connection. In contrast to these 1:2 sheet structures, honeaite does not appear to have dative
178 bonding; the only linkages between double-sheets are Tl-Au bonds.

179 It has been suggested that the short Te··Te distance of 2.84 Å in krennerite Au₃AgTe₈
180 may be associated with Te··Te inter-sheet bonding (Dye and Smyth, 2012). Indeed, no other
181 options appear to be possible for bonding between the sheets. Sylvanite AgAuTe₄, another
182 sheet structure, has a Te··Te inter-sheet distance of 2.89 Å. Calaverite AuTe₂, has a shortest
183 inter-sheet Te...Te distance of 3.20 Å. The shortest inter-sheet Te··Te and Te-Au distances in

184 honeaite are 4 Å, and as such are likely to be far too long to correspond to dative bonds.
185 Hence, the only significant inter-sheet bonding in honeaite is *via* the Tl-Au(2) bond (2.97 Å).

186 There are two synthetic silver-thallium-tellurides having an analogous Ag₃TlTe₂
187 stoichiometry: Ag₃TlTe₂ (Gelato et al. 1998) and Ag₁₈Tl₄Te₁₁ (Brun et al. 1992). Both have
188 very different structures from each other and from that of honeaite. Ag₃TlTe₂ (orthorhombic,
189 *Cmmm*) is an Ag-Te framework with strong compositional layering and Tl in [8]-
190 coordination Tl(Ag₄Te₄). Ag₁₈Tl₄Te₁₁ (cubic, *F43m*) is an Ag-Te framework with channels
191 occupied by Tl₆ octahedral clusters. In both compounds Te has high coordination ≥[6].

192 Finally, petzite Ag₃AuTe₂ (Haidinger 1845 cited by Frueh, 1959) and fischesserite
193 Ag₃AuSe₂ (Bindi and Cipriani, 2004) have the same 3:1:2 stoichiometry but very different
194 structures from that of honeaite.

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

201

202 **Acknowledgments**

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206 thanked for his efficient handling of the review process.

207

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240

241

242 **Figure Captions**

243 **Figure 1. (a)** The six-membered ring comprising fused chains of $\text{Te}(1)\text{Au}_3$ and $\text{Te}(2)\text{Au}_3$
244 pyramids. **(b)** A pair of $\text{Te}(1)\text{Au}_3$ and $\text{Te}(2)\text{Au}_3$ pyramids with Te-Au bond lengths shown.
245 The apex (Te) of the $\text{Te}(1)\text{Au}_3$ pyramid points up, that of the $\text{Te}(2)\text{Au}_3$ pyramid points down.
246 **(c)** connected six-membered rings forming a corrugated sheet composed of alternating rows
247 of $\text{Te}(1)\text{Au}_3$ and $\text{Te}(2)\text{Au}_3$ pyramids. **(d)** The same sheet as in (c) projected onto (001) and
248 showing the nature of the sheet corrugation.

249

250 **Figure 2. (a)** Polyhedral representation of the honeaite structure showing corrugated layers
251 composed of double-sheets of TeAu_3 pyramids with rows of thallium atoms (green spheres)

252 occupying grooves in sheet corrugations extending parallel to [001]. **(b)** A ball-and-spoke
253 representation of (a) showing Tl-Au bonds (dashed black lines), Tl...Te distances (dashed red
254 lines) and intra-sheet Au-Au bonds (solid blue lines).

255

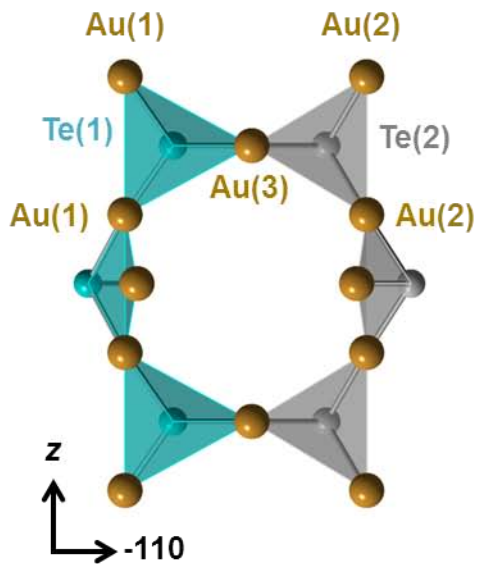
256 **Figure 3.** **(a)** Coordination and bond distances (Å) of Au and Tl atoms in honeaite. Au(1)
257 and Au(3) form octahedra, whereas Au(2) is four-coordinate, including an inter-sheet Au-Tl
258 bond (highlighted in red). Tl-Te distances are shown as dotted black lines and may not
259 correspond to real bonds. Anisotropic displacement parameters are drawn at the 68% level.
260 **(b)** Polyhedral connectivity of the three Au sites of honeaite. All atoms are drawn as spheres
261 and central Au sites are numbered.

262

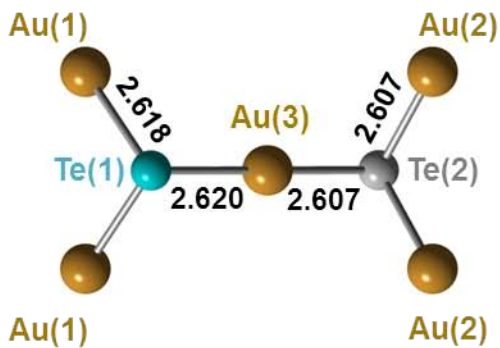
263 **Figure 4.** Fragment of the honeaite structure viewed slightly obliquely to the y axis and
264 showing the very different polyhedral connectivities of Te(1)Au₃ (blue) and Te(2)Au₃ (grey)
265 pyramids. Chains of TeAu₃ pyramids of the corrugated sheets extend parallel to [001]. For
266 each pyramid the Te atom is located at the apex that is not bonded to other polyhedra. TlAu₄
267 groups are shown green and each shares two edges with Te(1)Au₃ pyramids, making a fourth
268 longer inter-sheet bond to a Te(2)Au₃ pyramid of the adjacent double-sheet.

Figure 1

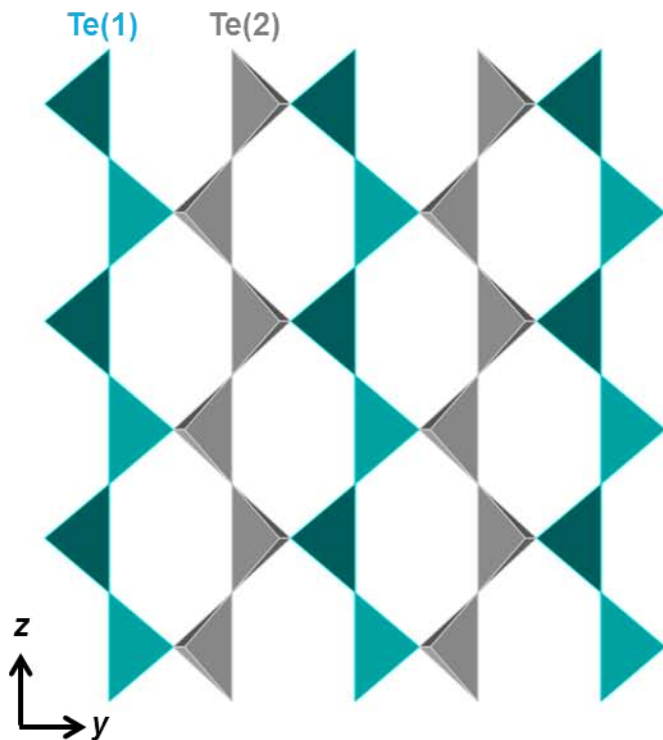
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(b)



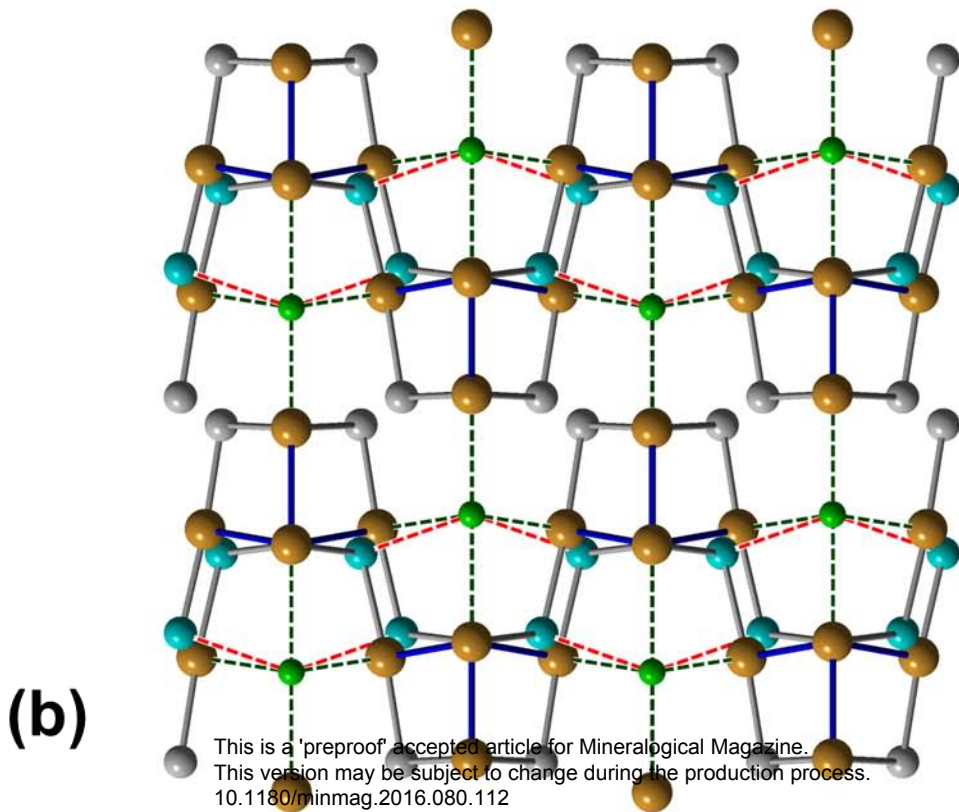
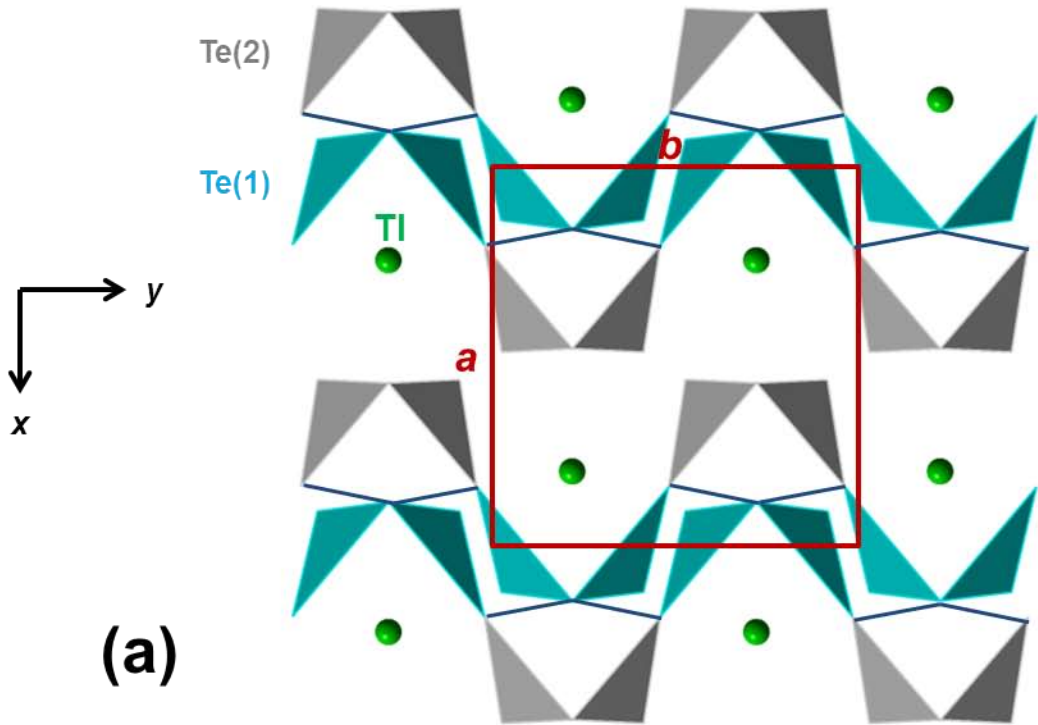
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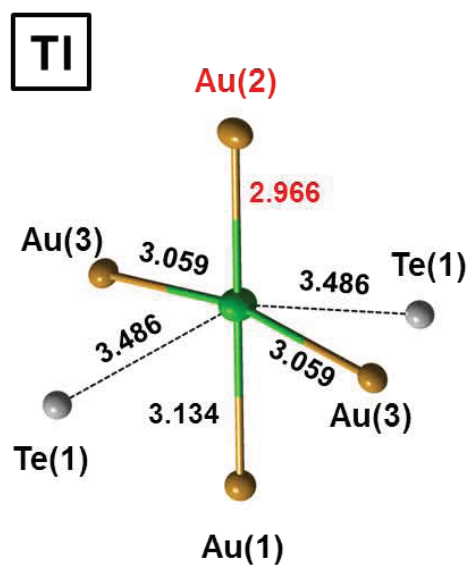
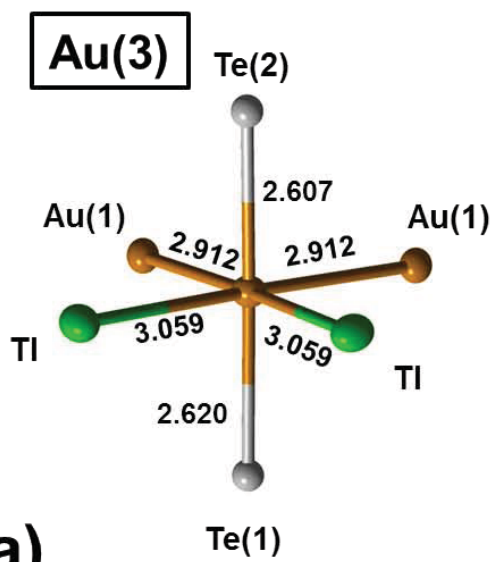
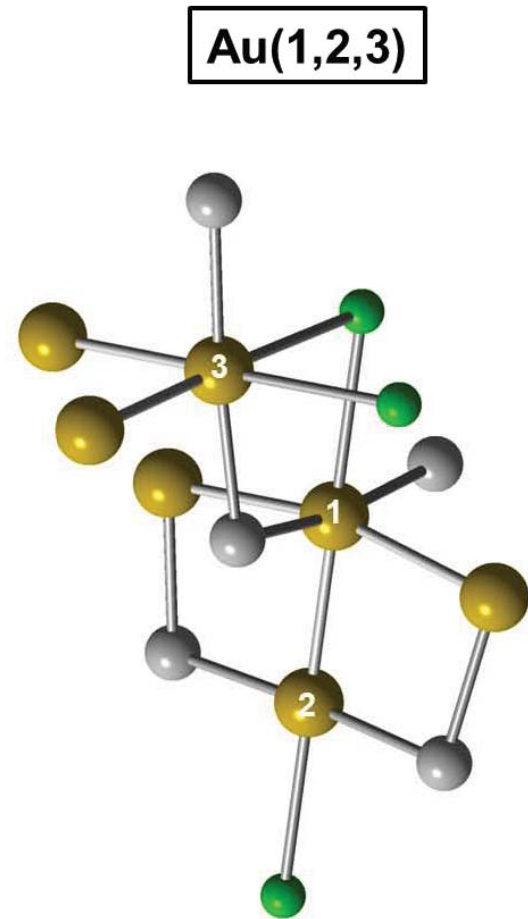
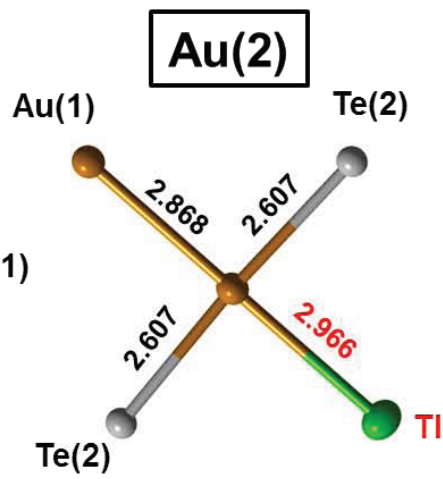
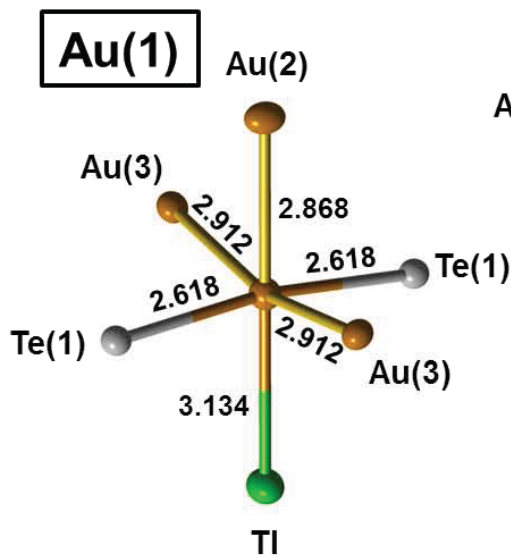


(d)

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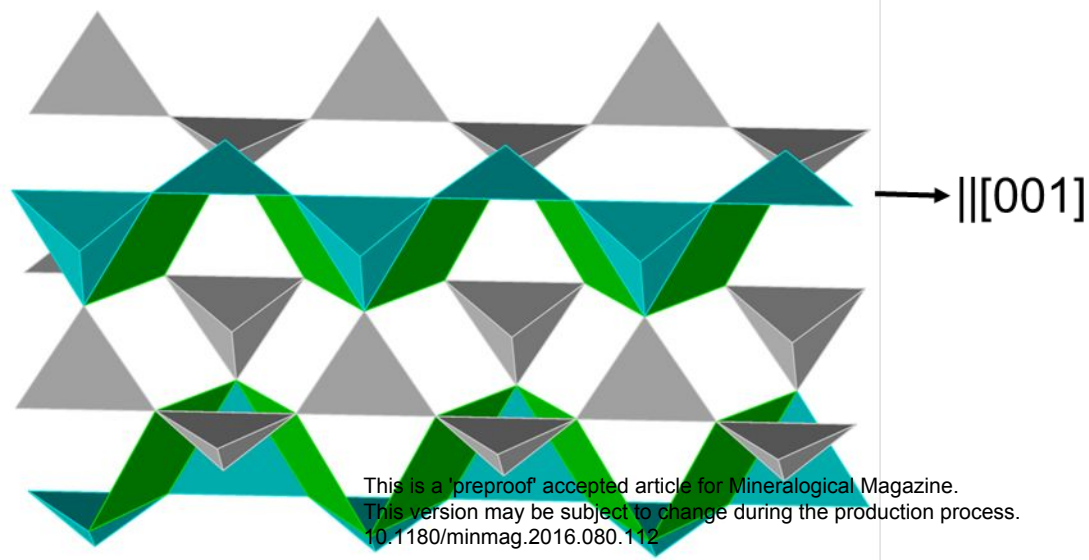
Figure 2





(a)

(b)



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

<i>Crystal data</i>	
Ideal chemical formula	Au ₃ TlTe ₂
Space group	<i>Pbcm</i>
<i>a</i> (Å)	8.9671(4)
<i>b</i> (Å)	8.8758(4)
<i>c</i> (Å)	7.8419(5)
<i>V</i> (Å ³)	624.14(6)
<i>Z</i>	4
<i>D_x</i> (Mg m ⁻³) calc	11.18
μ (mm ⁻¹)	105.05
<i>Data collection</i>	
Diffractometer	Xcalibur E (1K Eos detector)
Radiation, wavelength (Å)	MoK α , 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
<i>T</i> _{min} , <i>T</i> _{max}	0.233, 1
Reflections used for cell, <i>I</i> > 7 σ (<i>I</i>)	1903
Reflections measured	11673
<i>R</i> _{σ}	0.030
Independent reflections	1136
Independent reflections with <i>I</i> > 2 σ (<i>I</i>)	948
<i>R</i> _{int} (<i>mmm</i>)	0.058
θ _{min} , θ _{max} (°)	3.22, 31.91
Index range	-12 ≤ <i>h</i> ≤ 13, -12 ≤ <i>k</i> ≤ 13, -11 ≤ <i>l</i> ≤ 11
Data completeness to 30° θ (%)	99.9
<i>Refinement</i>	
Reflections, restraints, parameters	1136, 0, 34
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)], <i>R</i> ₁ (all)	0.033, 0.046
<i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)], <i>wR</i> ₂ (all)	0.050, 0.053
<i>GoF</i> (<i>F</i> ²)	1.087
Weighting scheme*	<i>a</i> = 0.0178
(Δ/σ) _{max}	<0.001
$\Delta\rho$ _{max} , $\Delta\rho$ _{min} (e Å ⁻³)	2.1, -3.6

* SHELX (Sheldrick, 2008)

Table 2. Atom coordinates and displacement parameters U^{ij} (\AA^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)	$\frac{3}{4}$	0	0.0196(3)	0.0263(3)	0.0255(3)	0.0043(2)	0	0	0.0238(1)
Au(1)	-0.13342(5)	$\frac{3}{4}$	0	0.0173(2)	0.0177(2)	0.0155(3)	0.0004(2)	0	0	0.0168(1)
Au(2)	0.54678(5)	$\frac{3}{4}$	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)	$\frac{1}{4}$	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)	$\frac{1}{4}$	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)	$-\frac{1}{4}$	0.0150(4)	0.0145(4)	0.0154(5)	0	0	0.0003(3)	0.0150(2)

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)		
