# Thunderbayite, $TlAg_3Au_3Sb_7S_6$, a new gold-bearing mineral from the Hemlo gold deposit, Marathon, Ontario, Canada

LUCA BINDI[1,2,*] and ANDREW C. ROBERTS[3]

[1]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Via G. La Pira 4, I-50121 Firenze, Italy
[2]CNR-Istituto di Geoscienze e Georisorse, Sezione di Firenze, Via G. La Pira 4, I-50121 Firenze, Italy
[3]Geological Survey of Canada, 601 Booth Street, Ottawa, Ontario, Canada KIA OE8

* e-mail: luca.bindi@unifi.it

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## ABSTRACT

Thunderbayite, ideally $TlAg_3Au_3Sb_7S_6$, is a new mineral from the Hemlo gold deposit, Marathon, Ontario, Canada. It occurs as very rare anhedral rims up to 70 μm across in contact with aurostibite and also spatially associated to stibarsen, biagioniite, and native gold in a calcite matrix. Thunderbayite is opaque with a metallic luster and shows a black streak. In reflected light, thunderbayite is weakly bireflectant and faintly pleochroic from grey-blue to slightly greenish grey-blue. Under crossed polars, it is weakly anisotropic with bluish to light-blue rotation tints. Internal reflections are absent. Reflectance percentages for the four COM wavelengths ($R_{min}$ and $R_{max}$) are 37.9, 38.4 (471.1 nm), 35.3, 36.0 (548.3 nm), 33.9, 34.4 (586.6 nm), and 32.0, 32.5 (652.3 nm), respectively. A mean of five electron-microprobe analyses gave Ag 14.91(16), Au 27.40(22), Tl 9.37(9), Sb 39.80(34), and S 8.61(7), for a total of 100.09 wt%, corresponding, on the basis of a total of 20 atoms, to $Tl_{1.00}Ag_{3.01}Au_{3.03}Sb_{7.12}S_{5.84}$. Thunderbayite is triclinic, space group $P1$, with $a$ = 8.0882(5), $b$ = 7.8492(5), $c$ = 20.078(1) Å, $\alpha$ = 92.518(5), β = 93.739(5), $\gamma$ = 90.028(6)°, $V$ = 1270.73(9) Å$^3$ and $Z$ = 2. The five strongest powder-diffraction lines [$d$ in Å ($I/I_0$) ($hkl$)] are: 4.04 (100)


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(200); 3.92 (80) (020); 2.815 (50) (220/-220); 2.566 (45) (-117); 2.727 (40) (0-17). The crystal structure [$R_1$ = 0.0220 for 5521 reflections with $I > 2\sigma(I)$] can be considered as a strongly deformed pyrite-type structure with several metal-metal bonds. Thunderbayite shows close similarities with criddleite, $TlAg_2Au_3Sb_{10}S_{10}$, from an optical, chemical and structural point of view. The new mineral has been approved by the IMA-CNMNC (No. 2020–042) and named for the Thunder Bay district (Ontario) in which the Hemlo gold deposit is located.

*Keywords*: thunderbayite, new mineral, thallium, criddleite, Hemlo deposit, Canada.

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## INTRODUCTION

In the course of a research project dealing with the description and structural characterization of natural Tl-Ag-sulfides/sulfosalts (i.e., Biagioni *et al.*, 2016; Bindi and Biagioni, 2018; Bindi *et al.*, 2012a, 2012b, 2013, 2015a, 2015b, 2020), we examined a sample from the Hemlo gold deposit, Marathon, Ontario, Canada (Harris, 1989), belonging to the mineralogical collections of the Museo di Storia Naturale of the University of Florence, Italy (catalogue number 46582/G). This is also the type material for the recently approved biagioniite, $Tl_2SbS_2$ (IMA 2019–120; Bindi and Moëlo, 2020). We were interested in the solution of the crystal structure of criddleite, $TlAg_2Au_3Sb_{10}S_{10}$ (Harris *et al.*, 1988), and tested several fragments by single-crystal X-ray diffraction. During this search, a few small grains turned out to be the new mineral thunderbayite, $TlAg_3Au_3Sb_7S_6$.

Thunderbayite was approved as a new mineral by the IMA-CNMNC (2020-042). The mineral name is for the Thunder Bay district (Ontario) in which the Hemlo gold deposit is located. The holotype material is deposited in the mineralogical collection of the Museo di Storia Naturale of the University of Florence (Italy), under catalog number 46582/G.

Here we report the description of the new mineral thunderbayite, together with its crystal structure.

## MATERIAL STUDIED

The sample containing thunderbayite, which is preserved in the collections of the Museo di Storia Naturale of the University of Florence, comes from the Hemlo gold deposit. Hemlo is an Archean-aged gold deposit located near the north-east shore of Lake Superior, about 35 km east of Marathon, Ontario, Canada and about 350 km east of Thunder Bay. The latitude and longitude co-ordinates are 48°41'41"N, 85°54'13"W. It is situated in the Hemlo-Schreiber greenstone belt of the Wawa sub-province of the Superior Province (Tomkins *et al.*, 2004, and references therein), and is located within a zone of strong deformation that essentially parallels the regional west-northwest trend and is stratiform within Archean-aged metamorphosed volcano-sedimentary rocks. The deposit has produced more than 21 Mozs of gold and consists of several mineralized zones in which the ore minerals were formed from hydrothermal fluids that is spatially related to the shear zone.

The sample consists of tiny thunderbayite grains up to 70 μm across spatially associated with aurostibite, stibarsen, biagioniite, and native gold in a calcite matrix. Thunderbayite was initially misidentified as criddleite.

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## PHYSICAL AND OPTICAL PROPERTIES

Thunderbayite occurs as very rare anhedral rims around aurostibite in a calcite matrix (Fig. 1). The mineral exhibits a subhedral to anhedral grain morphology, and does not show any inclusions of, or intergrowths with, other minerals. It is black in colour and shows a black streak. The mineral is opaque in transmitted light and exhibits a metallic luster. No cleavage is observed and the fracture is irregular. The calculated density (for $Z = 2$) for the empirical

formula (see below) is 5.693 g/cm$^3$. Unfortunately, the density could not be measured here because of the small grain size. The Mohs hardness, estimated with respect to the surrounding calcite (by scratching both minerals), is ~ 3.

In plane-polarized incident light, thunderbayite is grey in colour, weakly bireflectant and weakly pleochroic from grey-blue to slightly greenish grey-blue. Between crossed polars, thunderbayite is weakly anisotropic with bluish to light-blue rotation tints. Internal reflections are absent and there is no optical evidence of growth zonation.

Reflectance measurements were performed in air by means of a MPM-200 Zeiss microphotometer equipped with a MSP-20 system processor on a Zeiss Axioplan ore microscope. The filament temperature was approximately 3350 K. An interference filter was adjusted, in turn, to select four wavelengths for measurement (471.1, 548.3, 586.6, and 652.3 nm). Readings were taken for both the specimen and standard (SiC) maintained under the same focus conditions. The diameter of the circular measuring area was 0.04 mm. Reflectance percentages for $R_{min}$ and $R_{max}$ are 37.9, 38.4 (471.1 nm), 35.3, 36.0 (548.3 nm), 33.9, 34.4 (586.6 nm), and 32.0, 32.5 (652.3 nm), respectively.

In Figure 2, the reflectance values (measured in air) for criddleite ($TlAg_2Au_3Sb_{10}S_{10}$; Harris *et al.*, 1988), vaughanite ($TlHgSb_4S_7$; Harris *et al.*, 1989) and thunderbayite are compared. Although only a limited set of values (only for the four COM wavelengths) have been obtained for thunderbayite, it appears evident that its reflectance is similar to that of criddleite.

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## CHEMICAL COMPOSITION

A preliminary chemical analysis using EDS, performed on the crystal fragment used for the structural study, did not indicate the presence of elements (Z > 9) other than Ag, Au, Tl, Sb and S. Quantitative electron-microprobe analyses were carried out using a JEOL 8200

microprobe (WDS mode, 25 kV, 20 nA, 1 μm beam size, counting times 20 s for peak and 10 s for background). The following lines were used: Ag*L*α, Au*M*α, Tl*M*α, Sb*L*β, S*K*α. The standards employed were: synthetic TlI (Tl), Ag-pure element (Ag), Au-pure element (Au), synthetic $Sb_2Te_3$ (Sb) and pyrite (S). The crystal fragment was found to be homogeneous within analytical error. The average chemical compositions (5 analyses on different spots) together with wt% ranges of elements are reported in Table 1. On the basis of 20 atoms, the empirical formula of thunderbayite is $Tl_{1.00}Ag_{3.01}Au_{3.03}Sb_{7.12}S_{5.84}$. The ideal formula is $TlAg_3Au_3Sb_7S_6$, which requires Tl 9.45, Ag 14.96, Au 27.31, Sb 39.39, S 8.89, for a total 100 wt.%.

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## X-RAY CRYSTALLOGRAPHY AND CRYSTAL-STRUCTURE DETERMINATION

The same crystal fragment (20 × 20 × 30 μm) used to obtain the chemical data was selected for the X-ray single-crystal diffraction study that was done with a Bruker D8 Venture diffractometer equipped with a Photon II CCD detector, using graphite-monochromatised Mo *K*α radiation (λ = 0.71073 Å). Thunderbayite is triclinic, with $a$ = 8.088(3), $b$ = 7.854(3), $c$ = 20.078(8) Å, $\alpha$ = 92.52(3), β = 93.71(3), $\gamma$ = 90.15(4) °, $V$ = 1271.5(8) Å$^3$ and $Z$ = 2. Systematic absences were consistent with the space groups *P*1 and *P*-1. The statistical tests on the distribution of $|E|$ values ($|E^2-1|$ = 0.729) indicated the absence of an inversion center and so the *P*1 space group was chosen. The structure was solved and refined using the program SHELXL (Sheldrick, 2008). The occupancy of all the sites was left free to vary (Tl vs. □; Ag vs. □; Au vs. □; Sb vs. □; S vs. □) but all the positions were found to be fully occupied and then fixed in the subsequent refinement cycles. Neutral scattering curves for Tl, Ag, Au, Sb, and S were taken from the *International Tables for X-ray Crystallography* (Wilson, 1992). At the last stage, with anisotropic atomic displacement parameters for all the atoms and no

constraints, the residual value settled at $R_1$ = 0.0220 for 5521 observed reflections [2σ(*I*) level] and 361 parameters and at $R_1$ = 0.0245 for all 6799 independent reflections.

Experimental details and *R* indices are given in Table 2. Fractional atomic coordinates and atomic displacement parameters are reported in Table 3. Bond distances are given in Table 4. A CIF is deposited with the Principal Editor of Mineralogical Magazine at http://www.minersoc.org/pages/e_journals/dep_mat.html.

X-ray powder-diffraction data (Table 5) were collected with a Bruker D8 Venture diffractometer equipped with a Photon II CCD detector and using copper radiation (Cu *K*α, λ = 1.54138 Å). The program *Apex*3 (Bruker, 2016) was used to convert the observed diffraction rings to a conventional powder-diffraction pattern. The least squares refinement gave the following values: *a* = 8.0882(5), *b* = 7.8492(5), *c* = 20.078(1) Å, *α* = 92.518(5), β = 93.739(5), *γ* = 90.028(6) °, *V* = 1270.73(9) Å$^3$.

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## RESULTS AND DISCUSSION

### Description of the structure

In the crystal structure of thunderbayite there are two Tl sites, six Ag sites, six Au sites, 15 Sb sites, and 12 S sites. Noteworthy, the sites appear chemically pure, with no (or limited, if we consider the refinement uncertainties) substitutions. We cannot apply the classical crystal-chemical description that takes into account the metal-anion coordination polyhedra for thunderbayite, as several metal-metal bonds are present. Thallium atoms are three-fold coordinated by Sb, Ag/Au and S, with an additional contact with Sb at distance > 3.55 Å. By considering a limit < 3.4 Å for the coordination environment of Ag, Ag6 is three-fold coordinated, Ag1 and Ag4 are four-fold coordinated, Ag3 and Ag5 are six-fold coordinated, and Ag2 and Ag5 are seven-fold coordinated. Interestingly, all the Ag atoms coordinate Sb and S except Ag6, which shows a short bond with Tl2 equal to 2.803(3) Å.

Analogously, taking into account the same limit < 3.4 Å for the coordination environment of Au, all the Au atoms coordinate Sb and S except Au1, which shows a short bond with Tl1 equal to 2.920(2) Å. In detail, Au3 and Au4 are five-fold coordinated, Au1, Au5 and Au6 are six-fold coordinated and Au2 is seven-fold coordinated. The Sb atoms show several complex environments ranging from a three-fold to a six-fold coordination with Au/Ag, Sb and S. Only Sb1 and Sb11 make bonds with Tl, with distances varying from 2.889(5) Å (Sb1–Tl2) to 3.392(2) Å (Sb11–Tl1). Sb2, Sb6, Sb9 and Sb13 exhibit a similar coordination environment (five-fold coordination) with mean bond distances of 3.02, 3.08, 3.10 and 2.97 Å, respectively. Sb2 and Sb13 show close values of the mean bond distances as they coordinate to the same set of atoms: 2 Ag, 1 Au, and 2 S. Analogously, Sb6 and Sb9, having an almost identical coordination sphere, coordinate 2 Au, 1 Ag and 2 S atoms.

The crystal structure of thunderbayite can be viewed as a strongly deformed pyrite-type structure. It is well known that when half of the S atoms in pyrite-type compounds are replaced by other types of atoms, such as pnictogens, they can form different ordered ternary compounds, such as ullmannite (NiSbS)–type structures. The coordination environment of Ni in ullmannite (considering Sb and S as 'anions') closely resembles those observed (on average) for Ag and Au in thunderbayite (Figs. 3, 4 and Table 4). If we look at Figure 4, it appears that the structure of thunderbayite consists of *slabs* stacked along the **c**-axis: three alternate Au– and Ag–slabs with the Tl atoms terminating the unit-cell. The Au-slab is very similar to the Ni-slab in the crystal structure of ullmannite (Bayliss, 1977), with several Sb–S short bonds (Table 4). Therefore, thunderbayite might be regarded as an intergrowth structure of ternary pyrite-type slabs and Tl–Sb/S layers stacked along the **c**-axis.

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**Relationships between thunderbayite and criddleite**

Thunderbayite shows close similarities with criddleite, $TlAg_2Au_3Sb_{10}S_{10}$ (Harris *et al.*, 1988), from an optical, chemical and crystallographic point of view (very similar unit-cell values). As the two minerals come from the same mineral deposit, initially we thought thunderbayite and criddleite to be one and the same phase. However, the strongly different [Tl+Ag+Au]/(Sb+S) ratio (0.54 and 0.30 for thunderbayite and criddleite, respectively) and the differences in the strongest diffraction peaks [4.04(100), 3.92(90), 2.565(50) Å and 2.813(100), 5.63(90), 2.86(70) Å, for thunderbayite and criddleite, respectively] made us confident that they are different mineral species. Table 6 reports a comparison of the powder-diffraction data of thunderbayite and criddleite.

Although the crystal structure of criddleite is as yet unknown, it is very likely that it possesses the same metal–metal interactions as observed in thunderbayite. Similarly, also the unknown structure of vaughanite, $TlHgSb_4S_7$ (Harris *et al.*, 1989), might show the same features. However, discussions on charge balance, degree of metallic bonding and possible structural models must await the availability of suitable crystals for X-ray investigations.

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**TABLE AND FIGURE CAPTIONS**

Table 1. Electron-microprobe analysis (in wt% of elements) for thunderbayite

| Constituent | Mean | Range | Stand. Dev. (σ) |
|---|---|---|---|
| Ag | 14.91 | 14.79 – 15.03 | 0.16 |
| Au | 27.40 | 27.22 – 27.61 | 0.22 |
| Tl | 9.37 | 9.12 – 9.50 | 0.09 |
| Sb | 39.80 | 39.51 – 40.05 | 0.34 |
| S | 8.61 | 8.40 – 8.79 | 0.07 |
| Total | 100.09 | 99.09 – 100.16 | |

Table 2. Data and experimental details for the selected thunderbayite crystal

| | |
|---|---|
| **Crystal data** | |
| Formula | $TlAg_3Au_3Sb_7S_6$ |
| Crystal size (mm) | 0.020 × 0.020 × 0.030 |
| Form | block |
| Colour | black |
| Crystal system | triclinic |
| Space group | *P*1 (#1) |
| *a* (Å) | 8.088(3) |
| *b* (Å) | 7.854(3) |
| *c* (Å) | 20.078(8) |
| *α* (°) | 92.52(3) |
| *β* (°) | 93.71(3) |
| *γ* (°) | 90.15(4) |
| *V* (Å$^3$) | 1271.5(8) |
| *Z* | 2 |

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**Data collection**

| | |
|---|---|
| Instrument | Bruker D8 Venture |
| Radiation type | Mo$K\alpha$ ($\lambda$ = 0.71073) |
| Temperature (K) | 293(3) |
| Detector to sample distance (cm) | 6 |
| Number of frames | 1055 |
| Measuring time (s) | 50 |
| Maximum covered 2θ (°) | 67.48 |
| Absorption correction | multi-scan |
| Collected reflections | 18799 |
| Unique reflections | 6799 |
| Reflections with $F_o > 4\sigma(F_o)$ | 5521 |
| $R_{int}$ | 0.0208 |
| $R_\sigma$ | 0.0145 |
| Range of $h$, $k$, $l$ | $-7 \le h \le 9$, $-9 \le k \le 9$, $-30 \le l \le 30$ |

**Refinement**

| | |
|---|---|
| Refinement | Full-matrix least squares on $F^2$ |
| Final $R_1$ [$F_o > 4\sigma(F_o)$] | 0.0220 |
| Final $R_1$ (all data) | 0.0245 |
| Number refined parameters | 361 |
| GoF | 1.058 |
| $\Delta\rho_{max}$ (e Å$^{-3}$) | 0.56 |
| $\Delta\rho_{min}$ (e Å$^{-3}$) | -0.46 |

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Table 3. Atoms, atom coordinates and equivalent displacement parameters (Å$^2$) for thunderbayite

| atom | *x*/*a* | *y*/*b* | *z*/*c* | $U_{eq}$ |
|---|---|---|---|---|
| Tl1 | 0.51983(10) | 0.01613(9) | 0.98984(4) | 0.0874(2) |
| Tl2 | 0.48208(9) | 0.51764(9) | 0.04759(3) | 0.07683(19) |
| Ag1 | −0.01841(13) | −0.01304(12) | 0.23420(5) | 0.0506(2) |
| Ag2 | −0.01990(12) | −0.01104(11) | 0.52154(4) | 0.0431(2) |
| Ag3 | −0.0225(2) | −0.0150(2) | 0.81150(8) | 0.0932(4) |
| Ag4 | 0.47704(16) | 0.51585(16) | 0.33949(6) | 0.0694(3) |
| Ag5 | 0.48161(13) | 0.52001(13) | 0.60460(5) | 0.0520(2) |
| Ag6 | 0.4800(2) | 0.5239(2) | 0.90808(7) | 0.0919(4) |
| Au1 | 0.51393(9) | 0.01835(9) | 0.13515(4) | 0.07904(19) |
| Au2 | 0.51381(8) | 0.02540(8) | 0.42869(3) | 0.06754(17) |
| Au3 | 0.51237(6) | 0.02224(6) | 0.69923(2) | 0.04881(13) |
| Au4 | 0.01811(7) | 0.48143(7) | 0.14738(3) | 0.05465(15) |
| Au5 | 0.01606(8) | 0.48648(8) | 0.44131(3) | 0.06506(17) |
| Au6 | 0.01594(9) | 0.48543(9) | 0.70939(3) | 0.07471(19) |
| Sb1 | 0.62225(13) | 0.62812(13) | 0.17843(5) | 0.0636(3) |
| Sb2 | 0.62487(18) | 0.63013(18) | 0.46532(7) | 0.0897(4) |

| | | | | |
|---|---|---|---|---|
| Sb3 | 0.62270(15) | 0.62770(15) | 0.75223(6) | 0.0754(3) |
| Sb4 | 0.87755(14) | 0.35372(13) | 0.00921(5) | 0.0624(2) |
| Sb5 | 0.87418(13) | 0.37729(12) | 0.32541(5) | 0.0588(2) |
| Sb6 | 0.87037(16) | 0.37047(16) | 0.58138(6) | 0.0825(4) |
| Sb7 | 0.87271(12) | 0.37430(12) | 0.87835(4) | 0.0551(2) |
| Sb8 | 0.12319(17) | 0.87655(17) | 0.10718(6) | 0.0860(3) |
| Sb9 | 0.12482(14) | 0.87839(14) | 0.39822(5) | 0.0717(3) |
| Sb10 | 0.12395(13) | 0.87710(13) | 0.66835(5) | 0.0611(2) |
| Sb11 | 0.12450(11) | 0.87638(11) | 0.95727(4) | 0.0503(2) |
| Sb12 | 0.37074(14) | 0.12834(14) | 0.24922(5) | 0.0695(3) |
| Sb13 | 0.37429(12) | 0.12933(12) | 0.53772(4) | 0.0533(2) |
| Sb14 | 0.37250(19) | 0.12923(19) | 0.82125(7) | 0.0972(4) |
| S1 | 0.3705(7) | 0.3825(6) | 0.1687(2) | 0.0900(13) |
| S2 | 0.3752(5) | 0.3884(4) | 0.45807(16) | 0.0568(8) |
| S3 | 0.3827(4) | 0.3870(4) | 0.71542(14) | 0.0464(7) |
| S4 | 0.1269(6) | 0.6182(5) | 0.2757(2) | 0.0730(11) |
| S5 | 0.1230(7) | 0.6249(7) | 0.5723(2) | 0.0872(13) |
| S6 | 0.1251(4) | 0.6231(4) | 0.84379(14) | 0.0474(7) |
| S7 | 0.8750(3) | 0.1206(3) | 0.11298(12) | 0.0361(6) |
| S8 | 0.8792(7) | 0.1167(7) | 0.3989(3) | 0.0933(14) |
| S9 | 0.8795(5) | 0.1237(5) | 0.69460(19) | 0.0703(10) |
| S10 | 0.6162(6) | 0.8830(6) | 0.3086(2) | 0.0753(11) |
| S11 | 0.6170(5) | 0.8860(5) | 0.57502(17) | 0.0625(9) |
| S12 | 0.6227(5) | 0.8803(4) | 0.85802(16) | 0.0550(8) |

Table 4. Selected bond distances (Å) for thunderbayite

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Tl1- | Au1 | 2.920(2) | Au6- | Sb6 | 2.865(3) | S1- | Tl2 | 2.891(3) |
| | Sb11 | 3.392(1) | | Sb10 | 3.348(2) | | Au1 | 3.151(2) |
| | Sb14 | 3.663(2) | | S3 | 3.064(2) | | Au4 | 2.965(2) |
| | S12 | 2.979(2) | | S5 | 3.177(2) | | Sb1 | 2.793(3) |
| | | | | S6 | 2.943(3) | | Sb12 | 2.623(3) |
| Tl2- | Ag6 | 2.803(2) | | S9 | 3.041(2) | | | |
| | Sb1 | 2.889(3) | | | | S2- | Ag4 | 2.794(3) |
| | Sb4 | 3.569(2) | Sb1- | Tl2 | 2.889(5) | | Ag5 | 3.141(2) |
| | S1 | 2.891(3) | | Au1 | 3.327(3) | | Au2 | 3.113(4) |
| | | | | S1 | 2.793(2) | | Au5 | 3.009(2) |
| Ag1- | Sb8 | 2.959(2) | | S10 | 3.225(3) | | Sb2 | 2.761(3) |
| | Sb12 | 3.326(3) | | | | | Sb13 | 2.643(2) |
| | S4 | 3.251(2) | Sb2- | Ag4 | 2.832(3) | | | |
| | S7 | 2.780(4) | | Ag5 | 3.246(2) | S3- | Ag5 | 2.667(2) |
| | | | | Au2 | 3.334(4) | | Au3 | 3.064(3) |
| Ag2- | Sb6 | 3.323(2) | | S2 | 2.761(4) | | Au6 | 3.064(2) |
| | Sb9 | 2.906(4) | | S11 | 2.920(2) | | Sb3 | 2.750(3) |

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|---|---|---|---|---|---|---|---|---|
| | Sb10 | 3.256(2) | | | | | | |
| | Sb13 | 3.362(4) | Sb3- | Ag5 | 3.184(3) | S4- | Ag1 | 3.251(2) |
| | S5 | 3.267(2) | | S3 | 2.750(3) | | Ag4 | 3.153(3) |
| | S8 | 2.774(3) | | S12 | 2.842(2) | | Au4 | 2.833(2) |
| | S11 | 3.302(2) | | | | | Sb5 | 3.027(3) |
| | | | Sb4- | Au4 | 3.055(3) | | Sb9 | 3.129(2) |
| Ag3- | Sb10 | 3.258(2) | | Sb7 | 2.637(2) | | | |
| | Sb11 | 3.238(3) | | S7 | 2.835(3) | S5- | Ag2 | 3.267(2) |
| | Sb14 | 3.378(2) | | | | | Ag5 | 3.054(3) |
| | S6 | 3.163(3) | Sb5- | Au5 | 2.635(2) | | Au5 | 2.880(4) |
| | S9 | 2.704(2) | | S4 | 3.027(3) | | Au6 | 3.177(3) |
| | S12 | 3.192(3) | | S8 | 2.574(2) | | Sb6 | 2.874(2) |
| | | | | | | | Sb10 | 2.703(2) |
| Ag4- | Sb2 | 2.832(2) | Sb6- | Ag2 | 3.323(2) | | | |
| | S2 | 2.794(3) | | Au5 | 3.283(3) | S6- | Ag3 | 3.163(4) |
| | S4 | 3.153(2) | | Au6 | 2.865(4) | | Ag6 | 3.183(2) |
| | S10 | 3.193(5) | | S5 | 2.874(3) | | Au6 | 2.943(4) |
| | | | | S9 | 3.049(2) | | Sb7 | 2.958(3) |
| Ag5- | Sb2 | 3.246(2) | | | | | Sb11 | 2.958(2) |
| | Sb3 | 3.184(4) | Sb7- | Ag3 | 3.416(3) | | | |
| | Sb13 | 3.383(2) | | Sb4 | 2.637(2) | S7 | Ag1 | 2.780(3) |
| | S2 | 3.141(4) | | S6 | 2.958(3) | | Au1 | 3.092(3) |
| | S3 | 2.667(2) | | | | | Au4 | 3.091(2) |
| | S5 | 3.054(3) | Sb8- | Ag1 | 2.959(3) | | Sb4 | 2.835(2) |
| | S11 | 3.167(3) | | Au1 | 3.353(2) | | Sb8 | 2.784(4) |
| | | | | Au4 | 3.361(3) | | | |
| Ag6- | Tl2 | 2.803(3) | | Sb11 | 3.011(3) | S8- | Ag2 | 2.774(2) |
| | S6 | 3.183(2) | | S7 | 2.784(2) | | Au2 | 3.140(4) |
| | S12 | 3.249(3) | | | | | Au5 | 3.167(2) |
| | | | Sb9- | Ag2 | 2.906(3) | | Sb5 | 2.574(4) |
| Au1- | Tl1 | 2.920(2) | | Au2 | 3.358(2) | | Sb9 | 2.733(3) |
| | Sb1 | 3.327(4) | | Au5 | 3.364(5) | | S10 | 3.220(2) |
| | Sb8 | 3.353(4) | | S4 | 3.129(4) | | | |
| | Sb12 | 2.740(2) | | S8 | 2.733(2) | S9- | Ag3 | 2.704(2) |
| | S1 | 3.151(3) | | | | | Au3 | 3.081(3) |
| | S7 | 3.092(3) | Sb10- | Ag2 | 3.256(2) | | Au6 | 3.041(3) |
| | | | | Ag3 | 3.258(3) | | Sb6 | 3.049(4) |
| Au2- | Sb2 | 3.334(3) | | Au3 | 3.350(2) | | Sb10 | 2.829(2) |
| | Sb9 | 3.358(2) | | Au6 | 3.348(3) | | | |
| | Sb13 | 2.627(3) | | S5 | 2.703(2) | S10- | Ag4 | 3.193(2) |
| | S2 | 3.113(2) | | S9 | 2.829(4) | | Au2 | 2.789(2) |
| | S8 | 3.140(4) | | | | | Sb1 | 3.225(4) |
| | S10 | 2.789(2) | Sb11- | Tl1 | 3.392(2) | | Sb12 | 2.999(3) |
| | S11 | 3.240(2) | | Ag3 | 3.238(4) | | S8 | 3.220(2) |

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|---|---|---|---|---|---|---|---|---|
| | | | | Sb8 | 3.011(3) | | | |
| Au3- | Sb10 | 3.350(4) | | S6 | 2.958(2) | S11- | Ag2 | 3.302(3) |
| | Sb14 | 2.858(2) | | | | | Ag5 | 3.167(2) |
| | S3 | 3.064(3) | Sb12- | Ag1 | 3.326(2) | | Au2 | 3.240(3) |
| | S9 | 3.081(4) | | Au1 | 2.740(4) | | Au3 | 2.850(2) |
| | S11 | 2.850(2) | | S1 | 2.623(5) | | Sb2 | 2.920(4) |
| | | | | S10 | 2.999(2) | | Sb13 | 2.832(2) |
| Au4- | Sb4 | 3.055(3) | | | | | | |
| | Sb8 | 3.361(2) | Sb13- | Ag2 | 3.362(5) | S12- | Tl1 | 2.979(2) |
| | S1 | 2.965(4) | | Ag5 | 3.383(3) | | Ag3 | 3.192(4) |
| | S4 | 2.833(2) | | Au2 | 2.627(2) | | Ag6 | 3.249(3) |
| | S7 | 3.091(4) | | S2 | 2.643(3) | | Sb3 | 2.842(2) |
| | | | | S11 | 2.832(2) | | Sb14 | 2.901(3) |
| Au5- | Sb5 | 2.635(2) | | | | | | |
| | Sb6 | 3.283(4) | Sb14- | Ag3 | 3.378(3) | | | |
| | Sb9 | 3.364(2) | | Au3 | 2.858(2) | | | |
| | S2 | 3.009(3) | | S3 | 3.003(3) | | | |
| | S5 | 2.880(3) | | S12 | 2.901(2) | | | |
| | S8 | 3.167(2) | | | | | | |

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Table 5. Observed and calculated X-ray powder-diffraction data (*d* in Å) for thunderbayite.

| **1** | | | | | **2** | |
|---|---|---|---|---|---|---|
| $I_{calc}$ | $d_{calc}$ | *h* | *k* | *l* | $d_{meas}$ | $I_{meas}$ |
| 10 | 10.0082 | 0 | 0 | 2 | - | - |
| 18 | 6.6721 | 0 | 0 | 3 | 6.67 | 10 |
| 22 | 5.6414 | -1 | 1 | 0 | 5.63 | 30 |
| 11 | 5.6106 | 1 | 1 | 0 | | |
| 6 | 5.4492 | -1 | 1 | 1 | - | - |
| 9 | 5.0041 | 0 | 0 | 4 | 4.98 | 10 |
| 7 | 4.8862 | 1 | -1 | 2 | - | - |
| 9 | 4.4663 | -1 | -1 | 3 | - | - |
| 8 | 4.3370 | -1 | 1 | 3 | - | - |
| 9 | 4.3063 | 0 | -1 | 4 | 4.31 | 10 |
| 7 | 4.2794 | 1 | -1 | 3 | 4.21 | 15 |
| 11 | 4.1405 | 1 | 1 | 3 | | |
| 100 | 4.0355 | 2 | 0 | 0 | 4.04 | 100 |
| 90 | 3.9231 | 0 | 2 | 0 | 3.92 | 80 |
| 8 | 3.7690 | -1 | 1 | 4 | - | - |
| 12 | 3.7186 | 1 | -1 | 4 | 3.72 | 10 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 12 | 3.5998 | 1 | 1 | 4 | - | - |
| 33 | 3.5967 | -2 | 1 | 0 | 3.60 | 30 |
| 34 | 3.5807 | 2 | 1 | 0 | | |
| 12 | 3.5567 | -2 | 0 | 3 | - | - |
| 32 | 3.5360 | -1 | 2 | 0 | 3.53 | 30 |
| 28 | 3.5208 | 1 | 2 | 0 | - | - |
| 19 | 3.4492 | 0 | -2 | 3 | 3.44 | 15 |
| 9 | 3.3579 | 2 | 0 | 3 | 3.331 | 10 |
| 9 | 3.2625 | -2 | -1 | 3 | - | - |
| 11 | 3.2459 | -2 | 0 | 4 | | |
| 7 | 3.2168 | -2 | 1 | 3 | - | - |
| 12 | 3.2051 | -1 | -2 | 3 | - | - |
| 13 | 3.1559 | 0 | -2 | 4 | - | - |
| 15 | 3.1393 | 1 | -2 | 3 | 3.125 | 15 |
| 5 | 3.1174 | 2 | -1 | 3 | | |
| 11 | 3.1097 | -1 | 2 | 3 | - | - |
| 13 | 3.0462 | 2 | 0 | 4 | - | - |
| 10 | 3.0300 | 1 | 2 | 3 | - | - |
| 9 | 2.9763 | -1 | -2 | 4 | - | - |
| 7 | 2.9035 | 1 | -2 | 4 | - | - |
| 15 | 2.8595 | 0 | 0 | 7 | 2.860 | 10 |
| 37 | 2.8207 | -2 | 2 | 0 | 2.815 | 50 |
| 37 | 2.8053 | 2 | 2 | 0 | | |
| 9 | 2.7915 | 1 | 2 | 4 | 2.774 | 5 |
| 7 | 2.7521 | -1 | 0 | 7 | - | - |
| 49 | 2.7257 | 0 | -1 | 7 | 2.727 | 40 |
| 5 | 2.6903 | 3 | 0 | 0 | - | - |
| 22 | 2.6492 | 0 | 1 | 7 | 2.650 | 15 |
| 10 | 2.6419 | 1 | 0 | 7 | - | - |
| 7 | 2.6306 | -1 | -1 | 7 | - | - |
| 5 | 2.6108 | -2 | 2 | 3 | 2.612 | 5 |
| 54 | 2.5646 | -1 | 1 | 7 | 2.566 | 45 |
| 10 | 2.5532 | -3 | 0 | 3 | - | - |
| 7 | 2.5367 | 1 | -1 | 7 | - | - |
| 6 | 2.4921 | -1 | 3 | 0 | - | - |
| 6 | 2.4841 | 1 | 3 | 0 | - | - |
| 35 | 2.4721 | 1 | 1 | 7 | 2.473 | 30 |
| 9 | 2.4408 | 3 | 0 | 3 | - | - |
| 9 | 2.4363 | -3 | -1 | 3 | - | - |
| 5 | 2.4309 | 1 | -3 | 2 | - | - |
| 11 | 2.4196 | -3 | 1 | 3 | 2.420 | 10 |
| 5 | 2.3922 | 0 | 3 | 3 | - | - |
| 10 | 2.3766 | -1 | -3 | 3 | 2.375 | 10 |
| 10 | 2.3706 | 2 | 2 | 4 | - | - |
| 9 | 2.3516 | 1 | -3 | 3 | 2.351 | 10 |

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|---|---|---|---|---|---|---|
| 9 | 2.3447 | 3 | -1 | 3 | - | - |
| 16 | 2.3378 | -3 | -1 | 4 | 2.338 | 15 |
| 12 | 2.3243 | -2 | -1 | 7 | 2.325 | 10 |
| 8 | 2.3178 | -1 | 3 | 3 | - | - |
| 11 | 2.3168 | 3 | 1 | 3 | - | - |
| 15 | 2.3160 | -3 | 1 | 4 | 2.315 | 15 |
| 5 | 2.3079 | 3 | 0 | 4 | 2.306 | 5 |
| 8 | 2.2822 | 1 | 3 | 3 | 2.281 | 20 |
| 18 | 2.2820 | -1 | -3 | 4 | | |
| 16 | 2.2507 | 1 | -3 | 4 | 2.252 | 15 |
| 14 | 2.2293 | 3 | -1 | 4 | 2.227 | 10 |
| 12 | 2.2113 | -1 | 3 | 4 | - | - |
| 6 | 2.2003 | -2 | 3 | 0 | - | - |
| 13 | 2.1992 | 3 | 1 | 4 | 2.200 | 10 |
| 6 | 2.1893 | 2 | 3 | 0 | - | - |
| 10 | 2.1720 | 1 | 3 | 4 | - | - |
| 6 | 2.1241 | -1 | -1 | 9 | 2.124 | 5 |
| 13 | 2.0841 | -2 | -2 | 7 | - | - |
| 10 | 2.0261 | -3 | 0 | 7 | - | - |
| 7 | 2.0218 | -2 | 2 | 7 | - | - |
| 15 | 1.9946 | 2 | -2 | 7 | 1.995 | 15 |
| 12 | 1.9748 | -3 | -1 | 7 | 1.974 | 10 |
| 10 | 1.9588 | -2 | -1 | 9 | 1.959 | 10 |
| 5 | 1.9299 | 2 | 2 | 7 | - | - |
| 5 | 1.9085 | -1 | 4 | 0 | - | - |
| 7 | 1.8905 | -1 | -4 | 2 | - | - |
| 6 | 1.8805 | -3 | 3 | 0 | - | - |
| 10 | 1.8598 | 3 | -1 | 7 | - | - |
| 13 | 1.8585 | -1 | 3 | 7 | 1.857 | 10 |
| 6 | 1.8485 | 1 | -4 | 3 | - | - |
| 11 | 1.8203 | 1 | 3 | 7 | - | - |
| 8 | 1.7983 | -4 | 2 | 0 | - | - |
| 8 | 1.7903 | 4 | 2 | 0 | - | - |
| 7 | 1.7680 | -2 | 4 | 0 | - | - |
| 8 | 1.7604 | 2 | 4 | 0 | - | - |
| 5 | 1.7416 | 1 | -4 | 5 | - | - |
| 5 | 1.7274 | -4 | 1 | 6 | - | - |
| 5 | 1.7164 | -3 | 1 | 9 | - | - |
| 5 | 1.7007 | -2 | 0 | 11 | - | - |
| 5 | 1.6919 | -2 | -2 | 10 | - | - |
| 7 | 1.6793 | 0 | -2 | 11 | - | - |
| 5 | 1.6611 | -2 | 4 | 4 | - | - |
| 8 | 1.6477 | -3 | 3 | 6 | - | - |
| 5 | 1.6114 | -1 | 3 | 9 | - | - |
| 6 | 1.6233 | -3 | -3 | 7 | - | - |

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|---|---|---|---|---|---|---|
| 5 | 1.5891 | -3 | 4 | 0 | - | - |
| 5 | 1.5810 | -3 | 3 | 7 | - | - |
| 6 | 1.5615 | 3 | -3 | 7 | - | - |
| 5 | 1.5468 | -3 | 4 | 3 | - | - |
| 8 | 1.5365 | -4 | 3 | 4 | - | - |
| 5 | 1.4867 | 1 | -5 | 4 | - | - |
| 8 | 1.4238 | -1 | 0 | 14 | - | - |
| 5 | 1.4406 | -4 | -3 | 7 | - | - |
| 12 | 1.4103 | -4 | 4 | 0 | - | - |
| 12 | 1.4026 | 4 | 4 | 0 | - | - |

1: Calculated powder pattern and indexing for thunderbayite on the basis of $a$ = 8.088(3), $b$ = 7.854(3), $c$ = 20.078(8) Å, α = 92.52(3), β = 93.71(3), γ = 90.15(4)° and with the atom coordinates reported in Table 3 (only reflections with $I_{rel} \geq 5$ are listed).
2: observed diffraction pattern.

Table 6. X-ray powder-diffraction data ($d$ in Å) for thunderbayite compared to that of criddleite.

| **1** | | | | | **2** | |
|---|---|---|---|---|---|---|
| $I_{calc}$ | $d_{calc}$ | $h$ | $k$ | $l$ | $d_{meas}$ | $I_{meas}$ |
| 10 | 10.0082 | 0 | 0 | 2 | 10.01 | 5 |
| 18 | 6.6721 | 0 | 0 | 3 | 6.67 | 30 |
| 22 | 5.6414 | -1 | 1 | 0 | 5.63 | 90 |
| 11 | 5.6106 | 1 | 1 | 0 | | |
| 6 | 5.4492 | -1 | 1 | 1 | 5.45 | 10 |
| 9 | 5.0041 | 0 | 0 | 4 | 5.00 | 40 |
| | | | | | 4.94 | 5 |
| 7 | 4.8862 | 1 | -1 | 2 | 4.85 | 20 |
| 9 | 4.4663 | -1 | -1 | 3 | - | - |
| 8 | 4.3370 | -1 | 1 | 3 | 4.34 | 30 |
| 9 | 4.3063 | 0 | -1 | 4 | - | - |
| 7 | 4.2794 | 1 | -1 | 3 | 4.25 | 40 |
| 11 | 4.1405 | 1 | 1 | 3 | | |
| 100 | 4.0355 | 2 | 0 | 0 | 4.03 | 40 |
| | | | | | 4.00 | 15 |
| | | | | | 3.95 | 3 |
| 90 | 3.9231 | 0 | 2 | 0 | 3.91 | 50 |
| 11 | 3.8855 | -1 | -1 | 4 | | |
| 8 | 3.7690 | -1 | 1 | 4 | 3.75 | 1 |
| 12 | 3.7186 | 1 | -1 | 4 | 3.69 | 10 |
| 5 | 3.7087 | 0 | -2 | 2 | | |
| 12 | 3.5998 | 1 | 1 | 4 | - | - |
| 33 | 3.5967 | -2 | 1 | 0 | - | - |

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| | | | | | | |
|---|---|---|---|---|---|---|
| 34 | 3.5807 | 2 | 1 | 0 | - | - |
| 12 | 3.5567 | -2 | 0 | 3 | - | - |
| 32 | 3.5360 | -1 | 2 | 0 | - | - |
| 28 | 3.5208 | 1 | 2 | 0 | - | - |
| 19 | 3.4492 | 0 | -2 | 3 | 3.431 | 10 |
| 9 | 3.3579 | 2 | 0 | 3 | 3.331 | 10 |
| 9 | 3.2625 | -2 | -1 | 3 | 3.298 | 1 |
| 11 | 3.2459 | -2 | 0 | 4 | 3.225 | 3 |
| 7 | 3.2168 | -2 | 1 | 3 | | |
| 12 | 3.2051 | -1 | -2 | 3 | - | - |
| 13 | 3.1559 | 0 | -2 | 4 | - | - |
| 15 | 3.1393 | 1 | -2 | 3 | 3.142 | 5 |
| 5 | 3.1174 | 2 | -1 | 3 | | |
| 11 | 3.1097 | -1 | 2 | 3 | - | - |
| 13 | 3.0462 | 2 | 0 | 4 | - | - |
| 10 | 3.0300 | 1 | 2 | 3 | - | - |
| 9 | 2.9763 | -1 | -2 | 4 | - | - |
| 7 | 2.9035 | 1 | -2 | 4 | 2.896 | 5 |
| 15 | 2.8595 | 0 | 0 | 7 | 2.860 | 70 |
| 37 | 2.8207 | -2 | 2 | 0 | 2.813 | 100 |
| 37 | 2.8053 | 2 | 2 | 0 | | |
| 9 | 2.7915 | 1 | 2 | 4 | 2.774 | 3 |
| 7 | 2.7521 | -1 | 0 | 7 | - | - |
| 49 | 2.7257 | 0 | -1 | 7 | - | - |
| 5 | 2.6903 | 3 | 0 | 0 | 2.689 | 1 |
| 22 | 2.6492 | 0 | 1 | 7 | - | - |
| 10 | 2.6419 | 1 | 0 | 7 | - | - |
| 7 | 2.6306 | -1 | -1 | 7 | - | - |
| 5 | 2.6108 | -2 | 2 | 3 | 2.612 | 3 |
| 54 | 2.5646 | -1 | 1 | 7 | 2.569 | 30 |
| 10 | 2.5532 | -3 | 0 | 3 | 5.545 | 40 |
| 7 | 2.5367 | 1 | -1 | 7 | 2.522 | 15 |
| 6 | 2.4921 | -1 | 3 | 0 | 2.500 | 10 |
| 6 | 2.4841 | 1 | 3 | 0 | 2.480 | 30 |
| 35 | 2.4721 | 1 | 1 | 7 | 2.473 | 20 |
| 9 | 2.4408 | 3 | 0 | 3 | - | - |
| 9 | 2.4363 | -3 | -1 | 3 | - | - |
| 5 | 2.4309 | 1 | -3 | 2 | 2.426 | 3 |
| 11 | 2.4196 | -3 | 1 | 3 | - | - |
| 5 | 2.3922 | 0 | 3 | 3 | 2.392 | 3 |
| 10 | 2.3766 | -1 | -3 | 3 | 2.385 | 5 |
| 10 | 2.3706 | 2 | 2 | 4 | 2.366 | 10 |
| 9 | 2.3516 | 1 | -3 | 3 | 2.351 | 3 |
| 9 | 2.3447 | 3 | -1 | 3 | - | - |
| 16 | 2.3378 | -3 | -1 | 4 | - | - |

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| | | | | | | |
|---|---|---|---|---|---|---|
| 12 | 2.3243 | -2 | -1 | 7 | 2.329 | 1 |
| 8 | 2.3178 | -1 | 3 | 3 | - | - |
| 11 | 2.3168 | 3 | 1 | 3 | - | - |
| 15 | 2.3160 | -3 | 1 | 4 | - | - |
| 5 | 2.3079 | 3 | 0 | 4 | 2.305 | 5 |
| 8 | 2.2822 | 1 | 3 | 3 | 2.278 | 3 |
| 18 | 2.2820 | -1 | -3 | 4 | | |
| 16 | 2.2507 | 1 | -3 | 4 | - | - |
| 14 | 2.2293 | 3 | -1 | 4 | 2.225 | 5 |
| 12 | 2.2113 | -1 | 3 | 4 | - | - |
| 6 | 2.2003 | -2 | 3 | 0 | - | - |
| 13 | 2.1992 | 3 | 1 | 4 | - | - |
| 6 | 2.1893 | 2 | 3 | 0 | - | - |
| 10 | 2.1720 | 1 | 3 | 4 | - | - |
| 6 | 2.1241 | -1 | -1 | 9 | 2.125 | 10 |
| 13 | 2.0841 | -2 | -2 | 7 | - | - |
| 10 | 2.0261 | -3 | 0 | 7 | 2.030 | 30 |
| 7 | 2.0218 | -2 | 2 | 7 | 2.018 | 60 |
| 15 | 1.9946 | 2 | -2 | 7 | 2.001 | 3 |
| 12 | 1.9748 | -3 | -1 | 7 | 1.980 | 35 |
| 10 | 1.9588 | -2 | -1 | 9 | 1.959 | 70 |
| 5 | 1.9299 | 2 | 2 | 7 | 1.932 | 1 |
| 5 | 1.9085 | -1 | 4 | 0 | 1.909 | 5 |
| 7 | 1.8905 | -1 | -4 | 2 | 1.891 | 10 |
| 6 | 1.8805 | -3 | 3 | 0 | 1.873 | 10 |
| 10 | 1.8598 | 3 | -1 | 7 | - | - |
| 13 | 1.8585 | -1 | 3 | 7 | - | - |
| 6 | 1.8485 | 1 | -4 | 3 | 1.847 | 10 |
| 11 | 1.8203 | 1 | 3 | 7 | 1.815 | 1 |
| 8 | 1.7983 | -4 | 2 | 0 | 1.802 | 1 |
| 8 | 1.7903 | 4 | 2 | 0 | 1.793 | 15 |
| 7 | 1.7680 | -2 | 4 | 0 | - | - |
| 8 | 1.7604 | 2 | 4 | 0 | 1.761 | 10 |
| 5 | 1.7416 | 1 | -4 | 5 | 1.741 | 10 |
| 5 | 1.7274 | -4 | 1 | 6 | 1.726 | 10 |
| 5 | 1.7164 | -3 | 1 | 9 | 1.715 | 10 |
| 5 | 1.7007 | -2 | 0 | 11 | 1.697 | 3 |
| 5 | 1.6919 | -2 | -2 | 10 | 1.689 | 3 |
| 7 | 1.6793 | 0 | -2 | 11 | 1.679 | 3 |
| 5 | 1.6611 | -2 | 4 | 4 | 1.662 | 1 |
| 8 | 1.6477 | -3 | 3 | 6 | 1.648 | 30 |
| 5 | 1.6114 | -1 | 3 | 9 | 1.640 | 5 |
| 6 | 1.6233 | -3 | -3 | 7 | 1.620 | 3 |
| 5 | 1.5891 | -3 | 4 | 0 | 1.588 | 5 |
| 5 | 1.5810 | -3 | 3 | 7 | 1.580 | 5 |

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| | | | | | | |
|---|---|---|---|---|---|---|
| 6 | 1.5615 | 3 | -3 | 7 | 1.567 | 3 |
| 5 | 1.5468 | -3 | 4 | 3 | 1.548 | 3 |
| 8 | 1.5365 | -4 | 3 | 4 | 1.536 | 10 |
| 5 | 1.4867 | 1 | -5 | 4 | 1.486 | 5 |
| 8 | 1.4238 | -1 | 0 | 14 | 1.425 | 15 |
| 5 | 1.4406 | -4 | -3 | 7 | - | - |
| 12 | 1.4103 | -4 | 4 | 0 | 1.415 | 3 |
| 12 | 1.4026 | 4 | 4 | 0 | 1.399 | 40 |

1: Calculated powder pattern and indexing for thunderbayite on the basis of $a$ = 8.088(3), $b$ = 7.854(3), $c$ = 20.078(8) Å, $\alpha$ = 92.52(3), $\beta$ = 93.71(3), $\gamma$ = 90.15(4)° and with the atom coordinates reported in Table 3.
2: observed powder pattern reported for synthetic criddleite (Harris *et al.*, 1988).

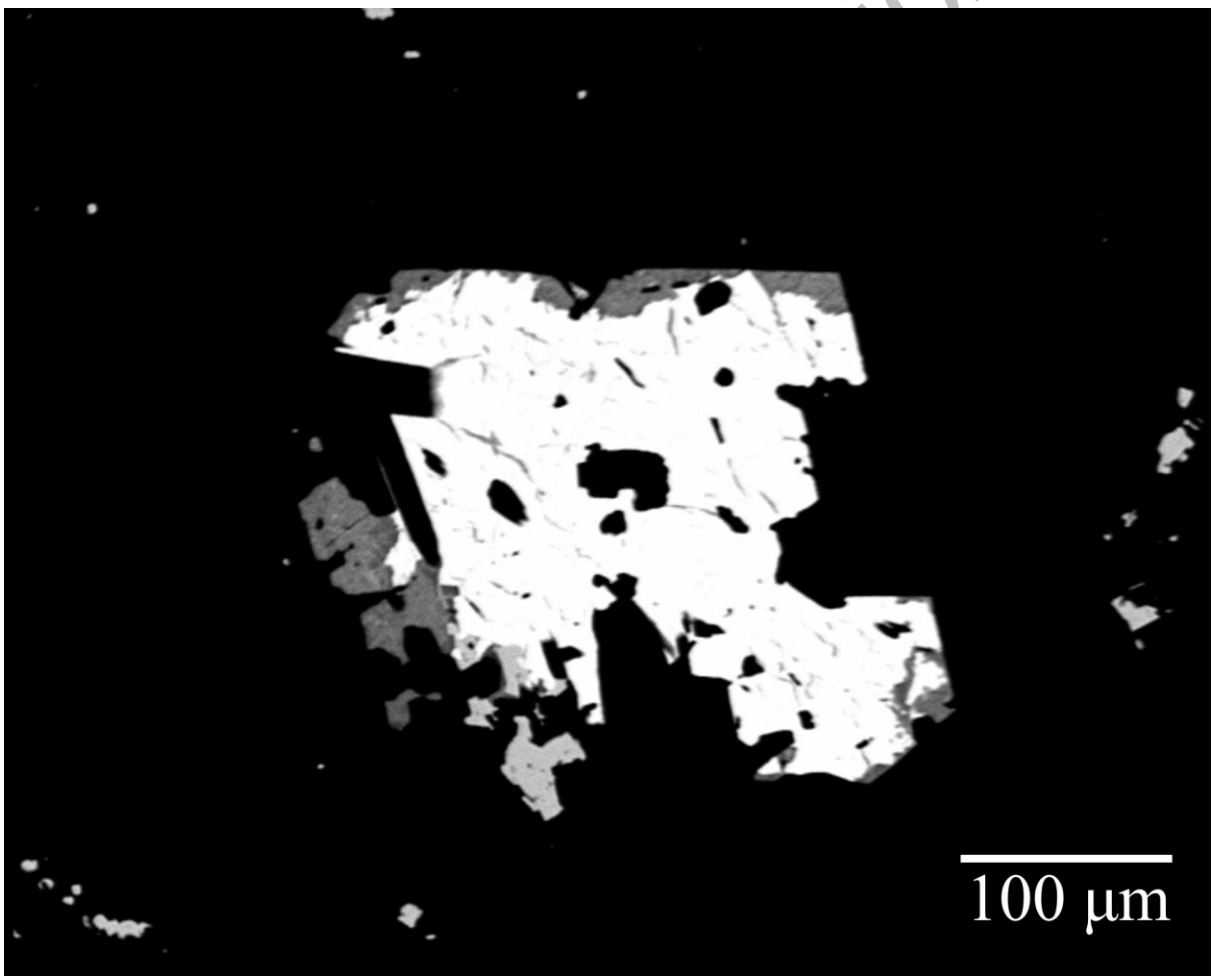


**FIGURE 1** – SEM-BSE image of thunderbayite (grey) associate with aurostibite (white) in a calcite matrix (black). The light grey phase at the bottom center is thunderbayite with a slightly higher Au/Ag ratio.

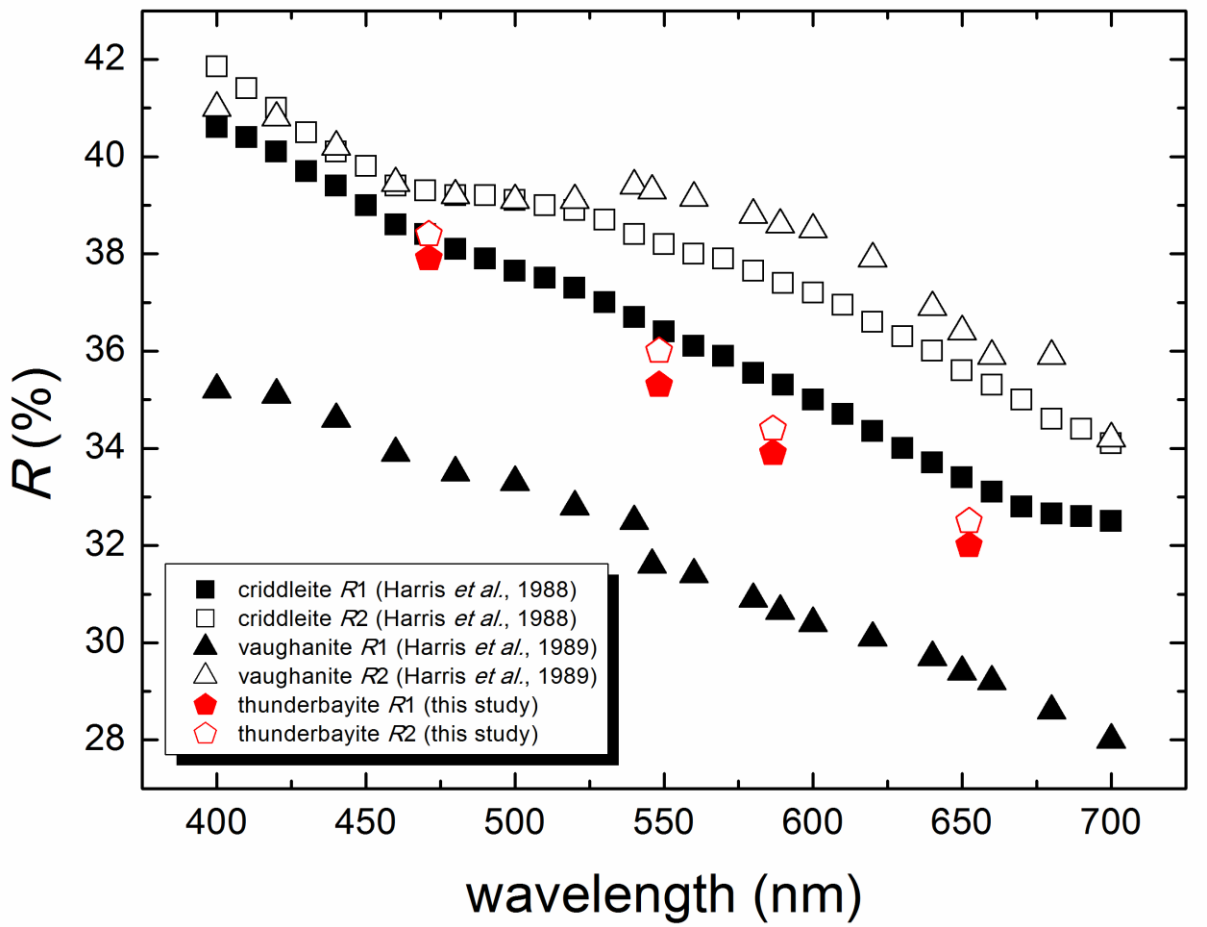


**FIGURE 2** – Reflectivity curves for thunderbayite in air (red symbols) compared to criddleite (black squares; Harris *et al.*, 1988) and vaughanite (black triangles; Harris *et al.*, 1989). Filled and open symbols refer to *R*1 and *R*2 values, respectively.

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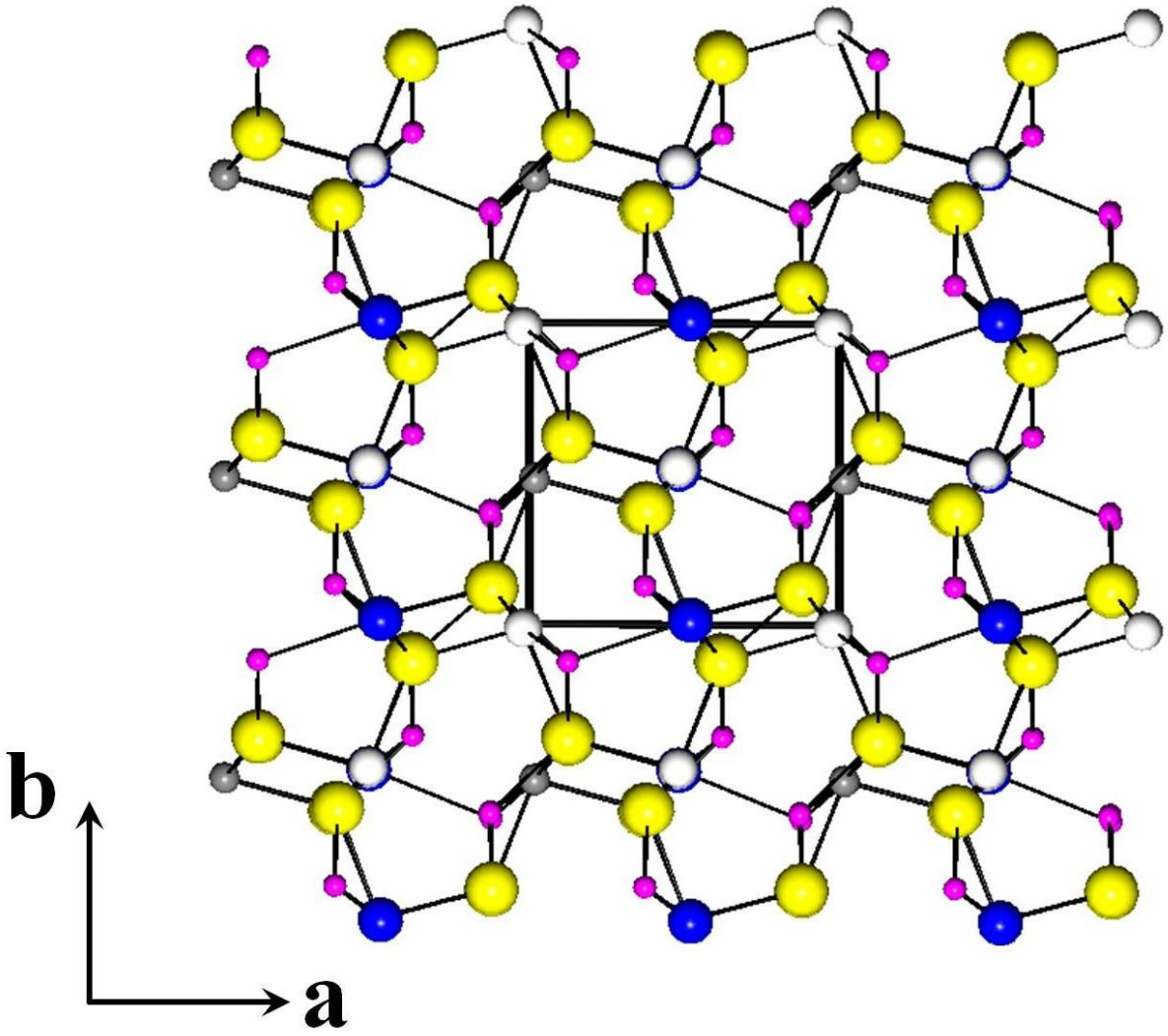


**FIGURE 3** – The crystal structure of thunderbayite down ~[001]. Tl, Ag, Au, Sb and S are given as blue, white, grey, violet and yellow circles, respectively. The unit-cell and the orientation of the structure are reported.

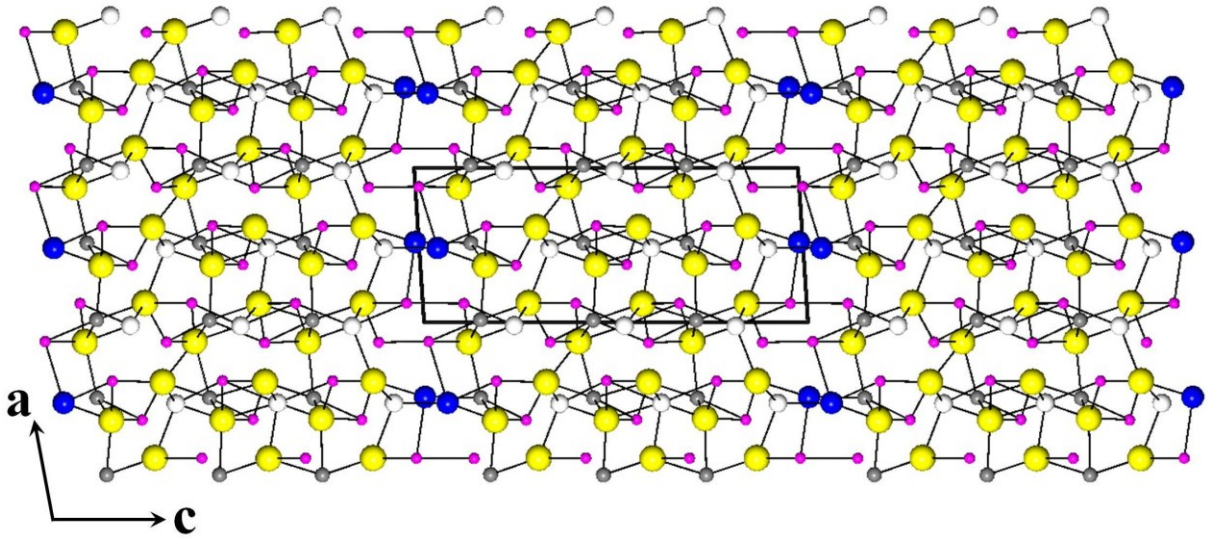


**FIGURE 4** – The crystal structure of thunderbayite down ~[010]. Symbols as in Figure 2. The unit-cell and the orientation of the structure are reported.