THE CRYSTAL STRUCTURE OF CHOLOALITE

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ABSTRACT

The crystal structure of choloalite, (Cu_{2.76}Sb_{6.21})(Pb_{2.19}Ca_{0.00})_6Te_{6.00}O_{18.09}Cl_{0.92}, a 12.520(4) Å, V 1963(2) Å^3, space group P4_32, Z = 4, has been solved by Patterson and direct methods, and refined to an R index of 5.3% based on 956 unique reflections measured using MoKα radiation on an automated four-circle diffractometer. The structure consists of distorted TeO_6 octahedra, Cu$S^5$ square pyramids (where $S$ = O and Cl), Pb(1)Oe triaugmented trigonal prisms, and Pb(2)O_{12} icosahedra. The Pb(1)Oe polyhedra polymerize to form a three-dimensional network, as do the CuO_4 square pyramids and Pb(2)O_{12} polyhedra. The two networks fit together in three-dimensional space, leaving voids that are filled by the TeO_6 octahedra. It is likely that the ideal formula of choloalite is CuPbTe_{4+2}O_6, with CuO_4 square planes as opposed to CuO_5 square pyramids.

Keywords: choloalite, crystal structure, tellurite, lead, copper.

INTRODUCTION

The type specimen of choloalite was described by Williams (1981) from waste rock in the tunnel at the Mina La Oriental, Moctezuma, Mexico. The type material consists of a matrix of intensely altered rhyolite vitrophyre crossed by veins of crystalline crusts and choloalite crystals. Soon after the discovery of the type material, samples with tiny crystals of choloalite were found between the dumps of the Joe and Grand Central shafts at Tombstone, Arizona. Choloalite also was described by Roberts et al. (1994) from the McAlpine mine, Tuolumne County, California.

The structure of choloalite was solved as part of a long-term project on the crystal chemistry of the Te-oxysalt minerals.

PREVIOUS WORK

Using powder X-ray-diffraction data, Williams (1981) showed that choloalite is isometric. The refined unit-cell dimensions were reported to be a 12.519 Å for the type specimen and 12.576 Å for the Tombstone sample. The larger cell edge of the Tombstone specimen was attributed to the presence of minor amounts of antimony. Wet-chemical analysis of the type material (Table 1) gave the empirical formula CuPb(Te_{4+2}O_{12})•H_2O.
The formula of choloalite was revised to \( \text{CuPb}(\text{TeO}_3)_2 \) by Powell et al. (1994), who synthesized crystals with this formula by fusion of stoichiometric amounts of \( \text{CuO}, \text{TeO}_2, \) and \( \text{PbO} \). No weight loss was detected with heating to 400°C, and infrared spectroscopy was used to confirm the absence of \( \text{H}_2\text{O} \). Powder X-ray-diffraction spectra of the synthetic material were found to be similar to those obtained from type choloalite, with some additional weak reflections. Powell et al. (1994) concluded that choloalite is anhydrous, and that the \( \text{H}_2\text{O} \) determined by Williams (1981), using only 156 \( \mu \text{g} \) of material, was adsorbed on the surface of the mineral particles. The cell dimension \( a \) obtained from the synthetic phase was 12.514 Å, and indexed reflections suggested possible space groups \( P2_132 \), \( P4321 \), \( P43m \), or \( Pm3m \) (none of which would result in systematic absences).

Powell et al. (1994) also suggested an additional occurrence of choloalite. This was based on the original description of balyakinite (Spiridonov 1980), which occurs with teinite and two unnamed \( \text{Cu}, \text{Pb} \) tellurites with formulae \( \text{CuPb}(\text{TeO}_3)_O \) and \( \text{CuPb}(\text{TeO}_3)_2 \) (as derived from electron-microprobe analyses). The latter formula is the same as that obtained by Powell et al. (1994) for their synthetic material.

**Experimental**

An electron-microprobe analysis was obtained using a JEOL 733 electron microprobe with Tracor Northern 5500 and 5600 automation. The wavelength-dispersion mode was used. The operating conditions were as follows: voltage 15 kV, beam current 20 nA, and beam diameter 5 \( \mu \text{m} \). Data for \( \text{Ca}, \text{Cu}, \text{Sb}, \) and \( \text{Te} \) were collected for 25 s; data for \( \text{Cl}, \text{Zn} \) and \( \text{Pb} \) were collected for 50 s. The following standards were used: scapolite (\( \text{ClK}_0 \)), \( \text{CaTaqO}_{11} \) (\( \text{CaK}_0 \)), cuprite (\( \text{CuK}_0 \)), \( \text{ZnWO}_4 \) (\( \text{ZnK}_0 \)), stibiotantalite (\( \text{SbLa}_0 \)), and \( \text{Pb}_2\text{TeO}_6 \) (\( \text{TeLa} \) and \( \text{PbMo} \)). Data were reduced using a PAP routine (program XMAQNT by C. Davidson, CSIRO). The results of the analysis are given in Table 1, together with the data of Williams (1981).

An attempt was made to obtain an infrared spectrum of choloalite, using a Fourier-transform infrared spectrometer equipped with a diamond-anvil microsample cell. The results show considerably more \( \text{H}_2\text{O} \) than could possibly be accommodated in the structure of choloalite. Since this is undoubtedly evidence of adsorbed \( \text{H}_2\text{O} \), the results of the infrared experiment were considered to be inconclusive.

The crystal used in this study is from the Mina La Oriental locality (Canadian Museum of Nature sample M158777). The crystal is optically isotropic and shows no evidence of twinning. It was mounted on a Siemens P3 automated four-circle diffractometer, and cell dimensions (Table 2) and intensity data were collected according to the procedure of Lam et al. (1998). One octant of reflections (3186 measurements, exclusive of standards) was collected from 3 to 60° 20; 64 reflections were rejected because of asymmetrical backgrounds, and one because of peak asymmetry. Fifteen strong reflections uniformly distributed with regard to 20 were measured at 5° intervals of \( \Psi \) (the azimuthal angle corresponding to rotation of the crystal about its diffraction vector) from 0 to 355°, after the method of North et al. (1968). These data (920 measurements) were used to calculate an absorption correction. The merging \( R \) index for the \( \Psi \)-scan data set decreased from 5.1% before the absorption correction to 2.1% after the absorption correction. This correction was then applied to the entire dataset; minimum and maximum transmissions were 0.88 and 0.68, respectively. The data were also corrected for Lorentz, polarization and background effects, averaged and reduced to structure factors. Of the 956 unique reflections, 455 were classed as observed \( [I \geq 3\sigma(I)] \).

**Structure Solution and Refinement**

The Siemens SHEXLTL PC system of programs was used throughout this study. Scattering curves for neutral atoms together with anomalous dispersion coefficients were taken from Cromer & Mann (1968) and Cromer & Liberman (1970). Miscellaneous data on the collection and refinement are given in Table 2.

| **TABLE 1. CHEMICAL COMPOSITION OF CHOLOALITE** |
|---|---|---|---|
| **Oxides** | **Williams (1981)** | **This study** | **Elements** | **Williams (1981)** | **This study** |
| CaO | trace | 0.50 | Ca²⁺ | trace | 0.17 |
| PbO | 33.0 | 31.22 | Pb²⁺ | 2.94 | 2.65 |
| CuO | 11.0 | 11.81 | Cu²⁺ | 2.75 | 2.81 |
| ZnO | — | 0.37 | Zn²⁺ | — | 0.09 |
| Sb₂O₅ | trace | 1.10 | Sb³⁺ | trace | 0.13 |
| TeO₂ | 50.7 | 51.81 | Te⁶⁺ | 6.31 | 6.15 |
| Cl | — | 1.19 | Cl⁻ | — | 0.64 |
| H₂O | 3.4 | — | — | 7.50 | — |
| CeCl₃ | — | — | — | 2.27 | — |
| TOTAL | 98.1 | 97.73 |

*Note: Analyses are normalized on 12 cations per formula unit.*

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**TABLE 2. MISCELLANEOUS INFORMATION: CHOLOALITE**

<table>
<thead>
<tr>
<th><strong>a (Å)</strong></th>
<th>12.520(4)</th>
<th>Rad/mono</th>
<th>MoKαgraphite</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu (Å^3) )</td>
<td>1063(2)</td>
<td>Total (</td>
<td>F_o</td>
</tr>
<tr>
<td>Space group</td>
<td>( P4_132 )</td>
<td>1 ( \geq 3\sigma(f) )</td>
<td>455</td>
</tr>
<tr>
<td>( Z )</td>
<td>4</td>
<td>( R ) (%)</td>
<td>5.3</td>
</tr>
<tr>
<td>Crystal size (mm)</td>
<td>0.04 \times 0.04 \times 0.05</td>
<td>( wR ) (%)</td>
<td>5.9</td>
</tr>
<tr>
<td>( \mu (\text{MoKα}; \text{mm}^{-1}) )</td>
<td>35.6</td>
<td></td>
<td></td>
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</table>

\( R = \sum|F_o| - |F_c| / \sum|F_o|, \quad wR = \left[ \sum w(F_o^2 - F_c^2)^2 / \sum wF_o^2 \right]^{1/2} \), \( w = 1 \)
The mean value of \(\langle E^2 - 1 \rangle\) was found to be 0.85, indicative of a non-centrosymmetric space-group. Systematic absences in the original dataset suggested the space groups \(P4_132\) and \(P4_13c\). The structure was solved by Patterson and direct methods and refined in \(P4_13c\) to an \(R\) index of 6.9% for an isotropic displacement model. The refined atomic positions were used in the normalization program STRUCTURE TIDY (Gelato & Parthé 1987), which suggested the enantiomorphic space-group \(P4_132\). The structure was refined in \(P4_13c\) to an \(R\) index of 6.9% for an isotropic displacement model. Conversion to anisotropic displacement factors for the oxygen atoms resulted in convergence at an \(R\) index of 6.9% for an isotropic displacement model. Conversion to anisotropic displacement factors for the oxygen atoms resulted in convergence at an \(R\) index of 5.1% (due to “smearing” of the electron density), but did not improve the model. Addition of an isotropic extinction correction did not improve the results. The program MISSYM (Le Page 1998) was used to search for additional elements of symmetry; none were indicated. Positional coordinates and anisotropic and equivalent isotropic displacement factors are given in Table 3. Interatomic distances and angles are given in Table 4, and a bond-valence analysis is in Table 5. Initially, bond-valence values were calculated using the curves of Brese & O’Keeffe (1991), but the sums were poor. Bond-valence values calculated using the “correction” terms given by Wang & Liebau (1996) for \(Te^{4+}\) were consistently too high. The curves of Brown (1981) were found to give the best sums for bonds to oxygen atoms (if the correct \(R\) value of 1.95 is used for \(Te^{4+}\), as shown by Back 1990). Structure factors may be obtained from the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario KIA 0S2, Canada.

**Description of the Structure**

Coordination polyhedra of cations in the choloalite structure are shown in Figure 1. There are four distinct cation positions in the structure. The \(Te\) site is completely occupied by \(Te^{4+}\), as shown by results of the electron-microprobe analysis, refined site-occupancy, and bond-valence analysis. The atom at the \(Te\) position is coordinated by at least four O atoms at distances of 1.87, 1.90, 1.92, and 2.71 Å. In accordance with Zemann (1968, 1971), Galy et al. (1975), and Effenberger et al. (1978), these can be described as forming a trigonal...
dipyramid, with a lone pair of electrons occupying one corner of the equatorial triangle. Brown (1974), however, assumed that the coordination environment of Te$^{4+}$ (and Sn$^{2+}$, Sb$^{3+}$, I$^{5+}$, and Xe$^{6+}$) is an octahedron distorted by a lengthening of some of the bonds on one side. Back (1990) showed that Te$^{4+}$ can be coordinated by up to eight anions, and Rossell et al. (1992) demonstrated that the coordination polyhedra of the four Te$^{4+}$ atoms in the structure of Bi$_2$Te$_4$O$_{11}$ can be described as distorted octahedra. In the crystal structure of choloalite, two additional O atoms, at distances of 2.95 and 3.05 Å, can be considered to form bonds with the atom at the Te position (contributing 0.16 and 0.13 valence units, $v_u$, respectively). The resulting polyhedron is a distorted octahedron, with three weak bonds occurring opposite three strong bonds. As suggested by Brown (1974), the bond-valence sum of each trans pair is approximately equal. The environment corresponds to type “C” of Brown (1974), although the valence ratio suggests configuration “A” (with two strong, two intermediate, and two weak bonds). The mean Te–O distance is 2.40 Å, and the O–Te–O angles range from 65.1 to 127.6°, with a mean value of 89°. The variance of the octahedron angle is 354.14, the mean quadratic elongation of the octahedron (Robinson et al. 1971) is 1.2296, and the polyhedron volume is 14.47 Å$^3$. The lone pair of electrons is most likely located on the side of the Te atom opposite the three closest O atoms, and within the volume defined by the Te atom and the three O atoms with the largest Te–O distances and O–Te–O angles. It is unlikely that the atom at the Te position forms a bond with the atom at the nearest Cl site, given the distance

<table>
<thead>
<tr>
<th>Table 5: Bond-Valence* Arrangement in Choloalite</th>
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<tbody>
<tr>
<td>Te</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>O(1)</td>
</tr>
<tr>
<td>O(2)</td>
</tr>
<tr>
<td>O(3)</td>
</tr>
<tr>
<td>Cl</td>
</tr>
<tr>
<td>Total</td>
</tr>
</tbody>
</table>

*Calculated from the curves of Brown (1981), as modified by Back (1990) for Te, and those of Brese & O’Keeffe (1991) for bonds to Cl.

Fig. 1. Coordination polyhedra of cations in the structure of choloalite. O atoms are shown as shadowed spheres, the Cl atom as an open, larger sphere.
trigonal prism. The Pb(1)-O distances are 2.46, 2.83, is coordinated by nine O atoms, forming a triaugmented fourfold coordination, and ll in fivefold coordination. by Eby & Hawthorne (1993), only three show Cu in the 94 Cu-oxysalt minerals listed in the compendium at the Cl position, and the true coordination would be longer, resulting in lower bond-valence sums. In this case, occupied by Cu, the bond distances would be slightly longer Sb. 

Then Sb at the Ca position is pentavalent. In addition, the chemical formulae obtained from both the electron-microprobe data suggest 92.7% Cu, 4.3% Sb, and 3.0% Zn at the Cu site (resulting in bond-valence sums of 2.33 and 2.34 vu for Sb4+ and Sb5+, respectively). The structure refinement shows 93(4)% Cu and 7(4)% Sb at the Cu position (resulting in bond-valence sums of 2.40 for both Sb4+ and Sb5+). Assuming no vacancies, the results show that the atom at the Cu site is overbonded by a minimum 0.26 vu. However, there is an additional site (labeled Cl) at a distance of 2.531 Å from the Cu position. The structure refinement shows that the Cl site is predominately occupied by Cl+. refinement of the site occupancy shows 92(12)% Cl at the Cl position, although the electron-microprobe data suggest only 0.64 Cl atoms per formula unit. There is no evidence for any other atom or molecule at the Cl position; as noted previously, the results of the infrared spectroscopy experiment were inconclusive as to the presence of OH or H2O. If the atom at the Cu position is considered to be bonded to one Cl atom in addition to four oxygen atoms, the resulting sphere of coordination is almost a square pyramid (actually a very distorted trigonal dipyramid), with a mean Cu–d (d: unspecified anion) distance of 2.02 Å, a mean O–Cu–d angle of 91.4°, and a polyhedron volume of 6.3 Å³.

It is likely that the Cl in choloalite serves to balance the excess positive charge introduced by Sb. Is the Sb at the Cu position trivalent or pentavalent? According to Shannon (1976), the ionic radii of Cu²⁺ and Sb⁵⁺ in fivefold coordination, and of Sb⁴⁺ in sixfold coordination, are 0.65, 0.80, and 0.60 Å, respectively. This suggests that the Sb at the Cu position is pentavalent. In addition, the chemical formulae obtained from both the electron-microprobe and crystal-structure analyses (see below) are only (approximately) charge-balanced with pentavalent Sb.

It is entirely possible that if the Cu site was only occupied by Cu, the bond distances would be slightly longer, resulting in lower bond-valence sums. In this case, there would be no need for additional negative charge at the Cl position, and the true coordination would be square-planar. However, it is interesting to note that of the 94 Cu-oxysalt minerals listed in the compendium by Eby & Hawthorne (1993), only three show Cu in fourfold coordination, and 11 in fivefold coordination.

The atom at the Pb(1) site, special position 8c (x,x,x), is coordinated by nine O atoms, forming a triaugmented trigonal prism. The Pb(1)–O distances are 2.46, 2.83, and 3.14 Å (all x3; mean 2.81 Å), and the O–Pb(1)–O angles range from 55.1 to 122.3° (mean 87.4°). The lengths of the polyhedron edges are 2.78, 3.07, 3.17, 3.18, 3.46, 3.74, and 3.92 Å (all x3). The polyhedron volume is 40.6 Å³. The coordination polyhedron is somewhat distorted, suggesting the presence of a lone pair of electrons. The results of the crystal-structure refinement show that the Pb(1) site is completely occupied by Pb⁺.

The atom at the Pb(2) site, special position 4a (3/8, 3/8,3/8), is coordinated by twelve O atoms, forming a distorted icosahedron. The Pb(2)–O distance range from 3.25 to 3.68 Å (both x3; mean 3.46 Å), and the O–Pb(2)–O angles range from 95.0 to 118.8° (mean 105.6°). The lengths of the polyhedron edges are 2.95 and 4.77 Å (both x3), and 2.76, 2.80, 3.17, and 3.37 Å (all x6). The polyhedron volume is 57.9 Å³. The structure refinement shows 72(1)% Pb and 28(1)% Ca at the Pb(2) position, which is in agreement with the electron-microprobe results (79% Pb and 21% Ca). Other minerals with twelve-coordinated Pb⁺ include osarizawaite (Giuseppetti & Tadini 1980), plumbojarosite (Szymalski 1985) and senaite (Grey & Lloyd 1976). All show six equal short and six equal longer Pb–O distances, with mean values of 2.82 to 2.92 Å. Although the Pb(2)–O distances in choloalite show a larger range, the mean value is close to those for the other minerals. It is difficult to describe a crystal structure as complicated as that of choloalite. We begin by assuming full occupancy of the CI position and a square-pyramidal coordination sphere around the atom at the Cu site (the alternate description, of a structure with a vacant Cl site and Cu with square-planar coordination, is only slightly different). We may consider the polymerization of coordination polyhedra by simple rotation around an atom (generally a central cation) at a special position. The Cl site, at special position 4b (7/8,7/8,7/8), lies at the intersection of one axis of twofold and one axis of threefold rotation. The atom at this site forms bonds with atoms at three Cu positions (each of which is on an axis of twofold rotation). Because of this, each Cu⁵⁺ square pyramid is attached to two others by corner-sharing of the atom or molecule at the Cl site, forming a “pinwheel” (Fig. 2a). In addition, each Cu⁵⁺ polyhedron shares two trans O(2)–O(3) edges (length 2.57 Å) with two TeO₆ octahedra, and the other trans O(2)–O(3) edges (length 2.76 Å) with two PbO₂₅ polyhedra. The lengths of the unshared O(2)–Cl and O(3)–Cl edges are 3.26 and 3.20 Å, respectively. In addition, each Cu⁵⁺ polyhedron is linked by corner-sharing to additional TeO₆ octahedra (×4) and Pb(1)O₆ polyhedra (×2).

The Pb(1) sites lie on axes of threefold rotation. Each Pb(1)O₆ polyhedron shares edges with three others, forming an additional “pinwheel” (Fig. 2b). The “pinwheels” polymerize to form a three-dimensional network (Fig. 3).

Like the Cl sites, the Pb(2) positions lie at intersections of one axis of twofold and one axis of threefold
Fig. 2. "Pinwheels" in the crystal structure of choloalite: (a) three Cu$_3$S$_5$ polyhedra; (b) four Pb(1)O$_9$ polyhedra; (c) seven Pb(2)O$_{12}$ polyhedra linked by six Cu$_3$S$_5$ polyhedra.

Fig. 3. Three-dimensional network of Pb(1)O$_9$ polyhedra. The Te atoms are shown as spheres. The positions of the 41 axes are evident.
rotation. Individual Pb(2)O₁₂ polyhedra are not joined; however, each is linked by the shared O(2)–O(3) edges to six Cu(2)₅ polyhedra. Each Cu(2)₅ polyhedron is then joined through the trans O(2)–O(3) edge to an additional Pb(2)O₁₂ polyhedron. The result is yet another “pinwheel” (Fig. 2c). These polymerize to form an additional three-dimensional network (Fig. 4).

The two three-dimensional networks are linked by the two trans O(2)–O(2)–O(2) faces (edge length 3.17 Å, ×3) of each Pb(2)O₁₂ icosahedron, which are shared with adjacent Pb(1)O₉ polyhedra. The spaces are filled with TeO₆ octahedra (note that the Te atom, alone among the cations in the choloalite structure, does not lie on an axis of rotation). The linkage of the TeO₆ polyhedra with neighboring polyhedra is shown in Figure 5. Each TeO₆ octahedron shares one triangular O(2)–O(3)–O(3) face with a Pb(2)O₁₂ polyhedron; the lengths of the shared edges are 2.80, 2.95, and 3.37 Å. In addition, each TeO₆ polyhedron shares one O(2)–O(3) edge (2.57 Å) with an adjacent Cu(2)₅ square pyramid, and one O(3)–O(3) (2.95 Å) and two O(1)–O(3) edges (2.96 × 2 Å) with three different TeO₆ octahedra. Furthermore, one O(1)–O(1) edge (3.18 Å) and one O(1)–O(2) edge (2.78 Å) are shared with adjacent Pb(1)O₉ polyhedra. The three unshared edges have lengths of 4.60, 4.81, and 5.08 Å. Finally, each TeO₆ polyhedron is linked by corner-
The empirical formula calculated from the chemical data is based on the structure analysis, which is electron-microprobe results, and calculated on the basis of the structure of copper oxysalt minerals. The empirical formula of choloalite, based on the electron-microprobe results, and calculated on the basis of the structure of copper oxysalt minerals is: 

\[ \text{Cu}_2 \text{Te}_6 \text{O}_{18} \text{Cl}_{10} \text{H}_2 \text{O} \]

This is similar to the formula based on the structure analysis, which is electron-microprobe results, and calculated on the basis of the structure of copper oxysalt minerals. The empirical formula calculated from the chemical data in Williams (1981) is: 

\[ \text{Cu}_2 \text{Te}_6 \text{O}_{18} \text{Cl}_{10} \text{H}_2 \text{O} \]

Our results show a Cl position that is approximately 64% occupied by Cl, which presumably is there to balance the excess positive charge introduced by Sb in the Cu site, and would not be present but for the Sb. Since there is no evidence to suggest that choloalite is normally a hydrous mineral, the ideal formula is likely CuPbTeO$_6$, as suggested by Powell et al. (1994).

Choloalite is one of five cubic Te-oxysalt minerals; the others are cliffordite, mcalpineite, winstanleyite, and yafsoanite. The structures of cliffordite and yafsoanite are known. Brandstätter (1981) showed that there are three distinct cation sites in the structure of cliffordite. The atom at the Te position, which is completely occupied by Te$^{2+}$, is coordinated by five Te$^{2+}$ octahedra with progressive crystallization. As noted previously, Williams (1981) derived the following paragenetic sequence from textural evidence: 

rodalquilarite → choloalite → emmonsite → cerussite.

The first three are all tellurites, suggesting that the oxidation potentials at the type locality were not high enough to produce Te$^{4+}$. The formula and crystal structure of yafsoanite are known. Brandstätter (1981) showed that it is a garnet-type structure, which could be associated with the stereochemistry of O and F complexes of Sn(II), Sb(III), Te(IV), I(V), and Xe(VI) J. Solid State Chem. 39, 1-8.

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