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BACKITE, $Pb_2Al(TeO_6)Cl$, A NEW TELLURATE MINERAL FROM THE GRAND CENTRAL MINE, TOMBSTONE HILLS, COCHISE COUNTY, ARIZONA: DESCRIPTION AND CRYSTAL STRUCTURE

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ABSTRACT

Backite, $Pb_2Al(TeO_6)Cl$, is a new tellurate mineral from the Grand Central mine, Tombstone Hills, Cochise County, Arizona. It occurs as rosettes of hexagonal plates perched on microcrystalline quartz, associated with schieffelinite, oboyerite, and rodalquilarite. Backite is dark to pale blue-grey, moderately transparent with opacity increasing with intensity of color, has a very pale bluish-grey streak, an adamantine luster, and does not fluoresce under ultraviolet light. It has a perfect micaceous cleavage parallel to {001}. Mohs hardness is 2–3, and backite is brittle with a splintery fracture. The calculated density is 5.573 g/cm^3. The indices of refraction are greater than 1.80, and grains are pleochroic in shades of blue-grey. Backite is trigonal, space group $P312$, a 5.0441(7), c 9.4210(5) Å, V 205.58(8) Å^3, $Z = 1$, c:a = 1:1.868. The six strongest lines in the X-ray powder diffraction pattern are as follows: d (Å), I, (h k l): 3.193, 100, (012); 4.363, 55, (010); 2.521, 55, (013, $\bar{1}20$); 1.555, 35, ($\bar{1}32$, 122); 1.978, 28, (022); 1.715, 20, (015, $\bar{1}24$, 114). Chemical analysis by electron microprobe gave TeO_3 24.05, Al_2O_3 7.07, PbO 63.74, S 1.15, Cl 2.28, O + Cl −1.09, sum 97.20 wt.% where the valence states of Te, Pb, and S were determined by crystal-structure analysis. The resulting empirical formula on the basis of 6 O anions is $Pb_{2.05}Al_{1.00}Te_{0.98}O_6(Cl_{0.46}S_{0.26})$ and the endmember formula is Pb_2AlTeO_6Cl. The crystal structure of backite was solved by direct methods and refined to an R_1 index of 4.20% based on 422 observed reflections collected with a three-circle rotating-anode diffractometer using Mo$K\alpha$ X-radiation. In the structure of backite, Te and Al octahedra occupy the vertices of a 6^3 net and each octahedron shares three edges with three adjacent octahedra. These layers of octahedra repeat along the **c** direction and are linked by a thick slab of lone-pair stereoactive Pb^{2+} cations and Cl^- anions. The structure is held together in the **c** direction by long, weak Pb–Cl bonds, accounting for the perfect cleavage parallel to {001}.

Keywords: Backite, new mineral species, tellurate, Grand Central mine, Tombstone Hills, Cochise County, Arizona, crystal structure, Raman spectrum.

INTRODUCTION

As part of our general interest in oxysalt minerals, we examined schieffelinite, $Pb_{10}Te_6O_{20}(OH)_{14}(SO_4)\cdot 5H_2O$ (Kampf *et al.* 2012), from the Grand Central mine, Tombstone, Arizona, USA. Associated with schieffelinite and yellow-green massive rodalquilarite is a dark blue-grey transparent mineral that occurs as rosettes of hexagonal plates. SEM-EDS analysis indicated the presence of Te, Pb/S/Mo, and O. The powder-diffraction pattern of the material did not match that of any known mineral, and subsequent solution of the crystal structure showed it to be a species new to science. The new mineral and mineral name were

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[§] *Corresponding author e-mail address*: frank.hawthorne@umanitoba.ca approved by the Commission on New Minerals, Nomenclature and Classification, International Mineralogical Association (IMA 2013-113). The mineral is named backite after Malcolm A. Back (born 1951), Department of Natural History (Mineralogy), Royal Ontario Museum, Toronto, Ontario. Malcolm Back has been involved in the description of several new minerals and is the principal author of *Fleischer's Glossary of Mineral Species 2008*. The holotype is deposited in the mineral collection of the Royal Ontario Museum, catalogue number M56436, and two cotype specimens are deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue numbers 64499 and 64500.

SAMPLE PROVENANCE

The specimens are from the Grand Central mine, Contention-Grand Central mine group, Tombstone District, Tombstone Hills, Cochise County, Arizona, USA. Grand Central mine is located ¾ mile south of Tombstone, Arizona. Oxidized Ag- and Au-bearing galena and minor copper and zinc ores occur in faulted and fractured parts of a dike, and in brecciated footwall zones of the dike. Backite occurs as rosettes of hexagonal plates perched on microcrystalline quartz, associated with schieffelinite, oboyerite, rodalquilarite, cerrusite, jarosite, and a new Pb-Cu tellurate-sulfate mineral.

PHYSICAL PROPERTIES

Backite crystals are hexagonal (trigonal) tablets up to 0.08 mm across, exhibiting the forms {100}, {010}, and {001} (Fig. 1). The faces of the basal pinacoid {001} form may be either flat and lustrous or rough; however, the faces of the trigonal prism forms {100} and {010} are invariably rough. Tablets occur as isolated individuals or in rosette-like intergrowths perched on quartz (Fig. 2), and are associated with cerussite, jarosite, and a new Pb-Cu tellurate-sulfate mineral; the rosettes are up to 0.15 mm in diameter. The megascopic color of the mineral is dark to pale blue-grey (Fig. 3) and crystals are moderately transparent with opacity increasing with intensity of color. The streak is white or very pale bluish gray, the luster is adamantine, and the mineral does not fluoresce under ultraviolet light. Crystals exhibit perfect micaceous cleavage parallel to {001}. The Mohs hardness is estimated at 2–3, the tenacity is brittle, and the fracture is splintery. The density of backite exceeds that of available density liquids and there is insufficient material for direct measurement; the calculated density is 5.573 g/cm^3. Backite is optically uniaxial negative. The indices of refraction are greater than 1.80. Efforts to measure the indices were

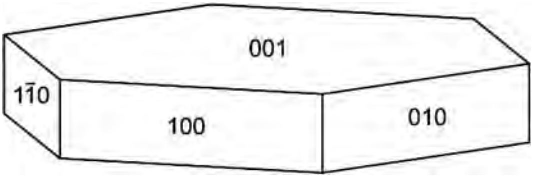

FIG. 1. Crystal drawing of backite (clinographic projection in standard orientation).

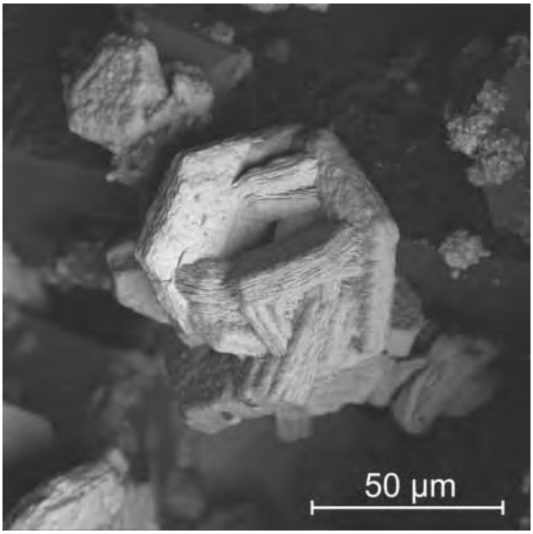

FIG. 2. Backscatter SEM image of a rosette of backite tablets on quartz.

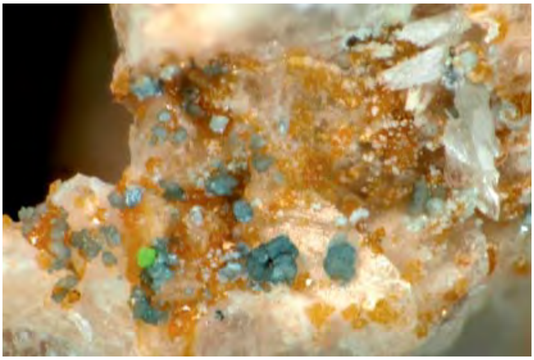

FIG. 3. Rosettes of bluish-grey backite on quartz associated with irregular white cerussite crystals (upper right), yellow-orange jarosite, and a lime-green rosette of a new Pb-Cu tellurate-sulfate mineral. Field of view is 2 mm.

unsuccessful because crystals are slowly attacked by index of refraction liquids greater than 1.80. The average index of refraction calculated using the Gladstone-Dale relation is 1.878. Crystals are pleochroic with O = bluish gray and E = colorless (O > E).

CHEMICAL COMPOSITION

Crystals were analyzed with a Cameca SX-100 electron microprobe operating in wavelength-dispersion mode with an accelerating voltage of 15 kV, a specimen current of 10 nA, and a beam diameter of 5 μm. The following standards were used: PbTe (Te, Pb), andalusite (Al), barite (S), and tugtupite (Cl). The data were reduced and corrected by the *PAP* method of Pouchou & Pichoir (1985). Table 1 gives the chemical composition (mean of three determinations). The empirical formula unit, based on 6 O atoms per formula unit (*pfu*), is $Pb_{2.05}Al_{1.00}Te_{0.98}O_6(Cl_{0.46}S_{0.26})$, the general formula is $Pb^{2+}_2AlTe^{6+}O_6(Cl^-,S^{2-},\square)$ and the endmember formula is $Pb^{2+}_2AlTe^{6+}O_6Cl$.

X-RAY POWDER DIFFRACTION

The powder-diffraction pattern of backite (Table 2) was recorded with a Bruker D8 Discover SuperSpeed micro-powder diffractometer with a HiStar multi-wire 2D detector using a modified Gandolfi attachment and Cu radiation (λ = 1.54178 Å) at 50 kV and 60 mA. Two 3h frames were merged, no internal standard was used, and the unit-cell parameters were refined by least squares, giving the following values: a = 5.043(1), c = 9.346(5) Å, V = 205.8(1) Å^3.

RAMAN SPECTROSCOPY

Raman spectra were acquired using a Horiba LabRAM Aramis micro-Raman spectrometer. A 785 nm, 100 mW laser was used, but was filtered to 1% power to prevent sample damage. A 1200 gr/mm grating and 100 μm slit were used during collection. A Si reference material was used for calibration. Two spectra were collected for 50 s at each point and the results were averaged. A 50× long-working-distance objective was used. Spectra were collected from 24 points on the sample and averaged to produce the final spectrum. Backite is not very Raman active (Fig. 4), and there are only slight frequency differences between Cl-dominant and S-dominant parts of the grains. Bands at 625 and 733 cm^{-1} are attributed to the symmetric and antisymmetric $Te^{6+}–O_6$ stretching modes, respectively, and the 425 cm^{-1} band to a $Te^{6+}–O_6$ bending mode (Frost & Keeffe 2008). The 350 cm^{-1} band is assigned to a Pb–Cl stretching mode and the 120 cm^{-1} band to a Cl–Pb–Cl bending mode (Frost & Williams 2004). The weak 967 cm^{-1} band is assigned to a combination band (*ca.* 350 + 625 cm^{-1}).

TABLE 1. CHEMICAL COMPOSITION (wt.%) AND ANALYTICAL DETAILS FOR BACKITE

Constituent	wt.%	Range	Electron Microprobe Standard
TeO_3	24.05	23.91–24.26	PbTe
Al_2O_3	7.07	6.97–7.15	andalusite
PbO	63.74	63.39–64.30	PbTe
S	1.15	1.07–1.24	barite
Cl	2.28	2.11–2.43	tugtupite
O = Cl	–1.09		
Total	97.20		

TABLE 2. POWDER-DIFFRACTION DATA FOR BACKITE

I_{rel}	d_{meas} (Å)	d_{calc} (Å)	$h\ k\ l$
7	9.303	9.346	0 0 1
2	4.667	4.673	0 0 2
55	**4.363**	4.367	0 1 0
11	**3.959**	3.957	0 1 1
100	**3.193**	3.191	0 1 2
55	**2.521**	2.522	1 1 0
2	2.435	2.434	1 1 1
4	2.340	2.336	0 0 4
8	2.223	2.219	1 1 2
17	**2.187**	2.184	0 2 0
3	2.126	2.126	0 2 1
5	2.059	2.060	0 1 4
28	**1.978**	1.978	0 2 2
10	1.961	1.960	$\bar{1}$ 2 3
20	**1.715**	1.718	0 1 5
		1.714	$\bar{1}$ 2 4
		1.714	1 1 4
9	1.651	1.651	$\bar{1}$ 3 0
3	1.625	1.626	$\bar{1}$ 3 1
3	1.594	1.595	0 2 4
35	**1.555**	1.556	$\bar{1}$ 3 2
		1.555	1 2 2

CRYSTAL-STRUCTURE SOLUTION AND REFINEMENT

A single crystal of backite (40 × 40 × 5 μm) was attached to a tapered glass fiber and mounted on a Bruker APEX II ULTRA three-circle diffractometer equipped with a rotating-anode generator (Mo*K*α), multilayer optics, and an APEX-II 4K CCD detector. A total of 2427 reflections was measured out to 60° 2θ using 6 s per 0.5° frame with a crystal-to-detector

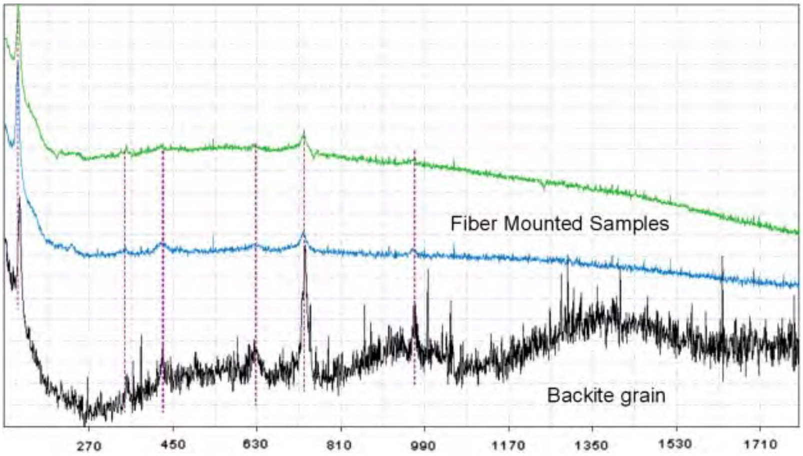

FIG. 4. The Raman spectrum of backite.

TABLE 3. MISCELLANEOUS INFORMATION FOR BACKITE

a (Å)	5.0441(7)	crystal size (μm)	5 × 40 × 40
c	9.4210(19)	radiation/monochromater	Mo$K\alpha$/Graphite
V (Å^3)	207.58(8)	No. of reflections	7799
Sp. Gr.	*P*312	No. in Ewald sphere	2427
Z	1	No. unique reflections	422
D_{calc} (g/cm^3)	5.573	R_{merge} %	3.49
Cell content	Pb_2AlTeO_6Cl	R_1 %	4.43
$R = \Sigma(\lvert F_o\rvert - \lvert F_c\rvert)/\Sigma\lvert F_o\rvert$		wR_2 %	12.23

$wR = [\Sigma w(|F_o|-|F_c|)^2/\Sigma F_o{}^2]^{1/2}$, $w = 1/[\sigma^2(F^2) + (0.0697 * P)^2 + 3.69 * P]$
where $P = [\mathrm{Max}(F_o{}^2, 0) + 2 * F_c{}^2]/3$

distance of 5 cm. Crystals invariably consist of partly divergent plates, and give large diffuse diffraction spots [hence the use of a wider (0.5°) than usual (0.2°) frame width to collect the diffraction data]. We attribute the extreme anisotropy of some of the observed displacement parameters to general structural disorder that reflects the divergent nature of the aggregates of plates. Unit-cell dimensions were determined by least-squares refinement of 4064 reflections with $I > 10\sigma I$, and are given in Table 3, together with other information pertaining to data collection and structure refinement. Empirical absorption corrections (SADABS; Sheldrick 2008) were applied and equivalent reflections were merged, resulting in 422 unique reflections, 422 of which were considered as observed [$|F_o| > 4\sigma F$].

All calculations were done with the SHELXTL PC (Plus) system of programs; *R* indices are of the form given in Table 3 and are expressed as percentages. Systematic absences in the single-crystal X-ray diffraction data are consistent with space group *P*312, and the structure was solved with this symmetry by direct methods and refined by full-matrix least-squares to an R_1 index of 4.43%. The site occupancies of the Cl(1) and Cl(2) sites were refined with the constraint that the sum of the occupancies be equal to the Cl and S contents indicated by chemical analysis (Table 1: Cl = 0.46, S = 0.26 *apfu*, expressed as equivalent Cl), and the isotropic-displacement parameters were constrained to be equal. Refined atom coordinates and anisotropic-displacement parameters are listed in Table 4 and selected interatomic distances are given in Table 5.

CRYSTAL STRUCTURE

Coordination of cations

In the structure, there is one *Te* site which the site scattering indicates is occupied by Te in octahedral coordination by O with a <Te–O> distance of 1.921 (9) Å, characteristic of Te^{6+}. There is one *Al* site octahedrally coordinated by O, with an <Al–O>

TABLE 4. ATOM POSITIONS AND ANISOTROPIC-DISPLACEMENT PARAMETERS FOR BACKITE

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Al	⅔	⅓	½	0.011(3)	0.011(3)	0.007(5)	0	0	0.0055(14)	0.010(2)
Te	0	0	½	0.0003(4)	0.0003(4)	0.050(2)	0	0	0.0002(2)	0.0167(9)
Pb	⅓	⅔	0.23936(10)	0.0186(4)	0.0186(4)	0.0303(4)	0	0	0.0093(2)	0.0225(3)
O(1)	0.336(2)	0.0379(19)	0.3883(10)	0.005(3)	0.009(5)	0.039(4)	−0.004(3)	0.001(4)	0.003(3)	0.0187(16)
Cl(1)	⅔	⅓	0	0.058(7)						
Cl(2)	0	0	0	0.058(7)						

TABLE 5. SELECTED INTERATOMIC DISTANCES (Å) IN BACKITE

Te–O(1) ×6	1.921(9)	Pb–O(1) ×3	2.335(9)
		Pb–Cl(1) ×3	3.683(1)
Al–O(1) ×6	1.904(9)	Pb–Cl(2) ×3	3.683(1)

distance of 1.904(9) Å and a site-scattering value characteristic of Al. There is one *Pb* site, which the site scattering indicates is occupied by Pb in [9]-coordination by three O and six Cl atoms with a <Pb–O> distance of 2.335(9) Å and <Pb–Cl> distances of 3.683(1) Å, characteristic of Pb^{2+}. This very asymmetric coordination of Pb^{2+} indicates that it is lone-pair stereoactive; details of this behavior in a wide range of compounds have been summarized by Shimoni-Livny *et al.* (1998).

Structure topology

The Te and Al octahedra occupy the vertices of a 6^3 net and each octahedron shares three edges with three adjacent octahedra (Fig. 5). These layers of octahedra repeat along the **c** direction (Fig. 6) and are linked by a thick slab of Pb^{2+} cations and Cl^- anions. Each Pb^{2+} cation bonds to three O^{2-} anions at short distances on one side, and to six Cl^- anions at long distances on the other side. The slab consists of a central layer of Cl^- anions and two sandwiching layers of Pb^{2+} cations (Fig. 6); when viewed down the **c** direction, each Pb^{2+} cation overlies a vacancy in the layer of octahedra and each Cl^- anion overlies an occupied octahedron in the layer of octahedra. The structure is held together in the **c** direction by long, weak Pb–Cl bonds, accounting for the good cleavage parallel to {001}.

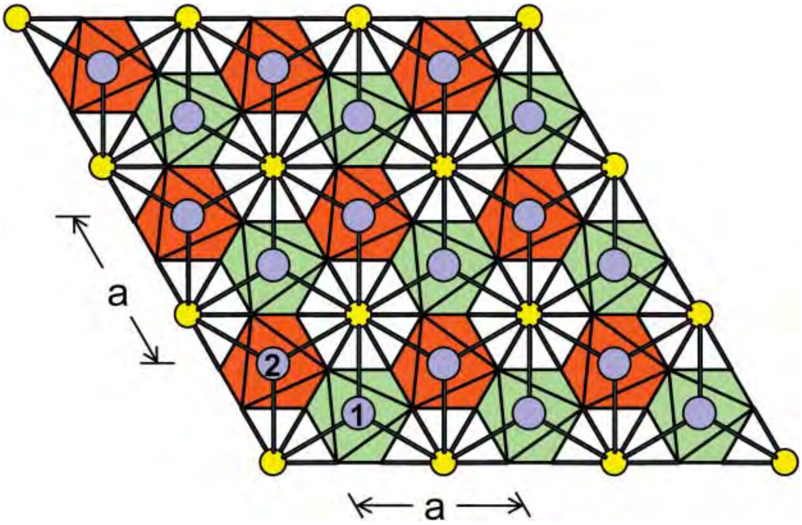

FIG. 5. The crystal structure of backite viewed down **c**; Al octahedra are green, Te octahedra are orange, Pb atoms are yellow circles, Cl atoms are blue circles and are numbered, Pb–(O,Cl) bonds are shown as thick black lines.

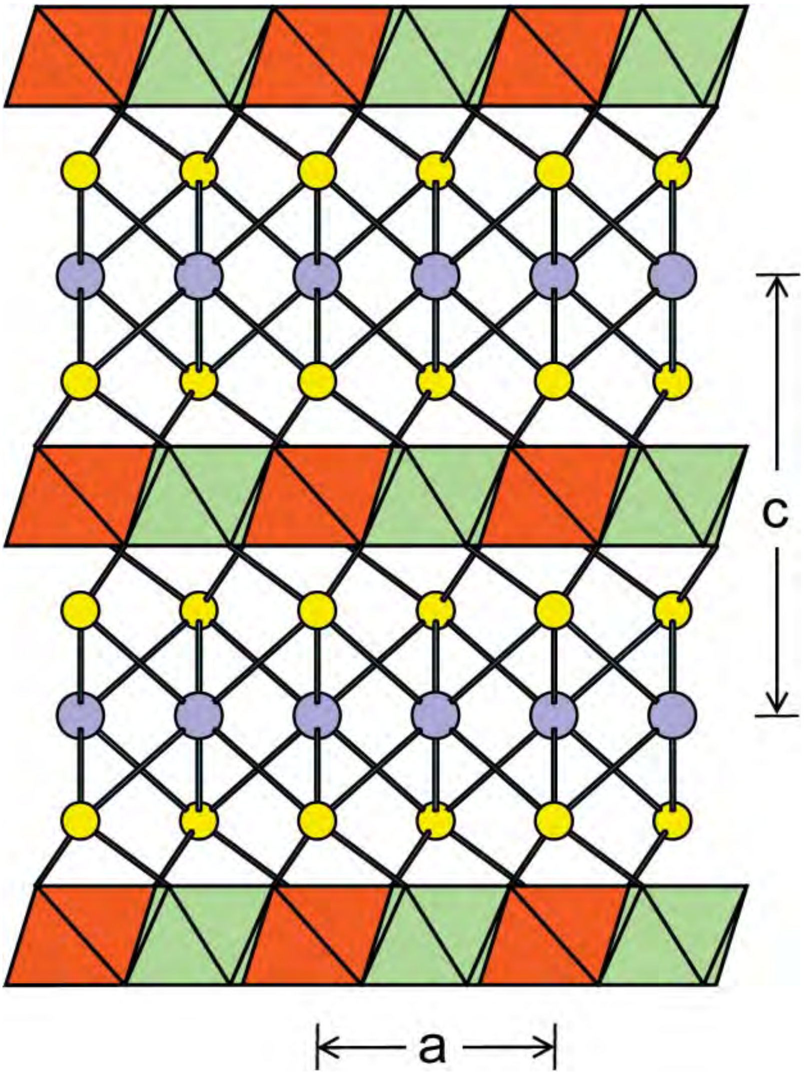

FIG. 6. The crystal structure of backite viewed perpendicular to **c**; legend as in Figure 5.

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