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Bobmeyerite, a new mineral from Tiger, Arizona, USA, structurally related to cerchiaraite and ashburtonite

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ABSTRACT

Bobmeyerite, $Pb_4(Al_3Cu)(Si_4O_{12})(S_{0.5}Si_{0.5}O_4)(OH)_7Cl(H_2O)_3$, is a new mineral from the Mammoth–Saint Anthony mine, Tiger, Pinal County, Arizona, USA. It occurs in an oxidation zone assemblage attributed to progressive alteration and crystallization in a closed system. Other minerals in this assemblage include atacamite, caledonite, cerussite, connellite, diaboleite, fluorite, georgerobinsonite, hematite, leadhillite, matlockite, murdochite, phosgenite, pinalite, quartz, wulfenite and yedlinite. Bobmeyerite occurs as colourless to white or cream-coloured needles, up to 300 μm in length, that taper to sharp points. The streak is white and the lustre is adamantine, dull or silky. Bobmeyerite is not fluorescent. The hardness could not be determined, the tenacity is brittle and no cleavage was observed. The calculated density is 4.381 g cm^{-3}. Bobmeyerite is biaxial (−) with $\alpha \approx \beta = 1.759(2)$, $\gamma = 1.756(2)$ (white light), it is not pleochroic; the orientation is X = **c**; Y or Z = **a** or **b**. Electron-microprobe analyses provided the empirical formula $Pb_{3.80}Ca_{0.04}Al_{3.04}Cu^{2+}_{0.96}Cr^{3+}_{0.13}Si_{4.40}S_{0.58}O_{24.43}Cl_{1.05}F_{0.52}H_{11.83}$. Bobmeyerite is orthorhombic (pseudotetragonal), *Pnnm* with unit-cell parameters $a = 13.969(9)$, $b = 14.243(10)$, $c = 5.893(4)$ Å, $V = 1172.5(1.4)$ Å^3 and $Z = 2$. The nine strongest lines in the X-ray powder diffraction pattern, listed as [d_{obs}(Å)(I)(hkl)], are as follows: 10.051(35)(110); 5.474(54)(011,101); 5.011(35)(220); 4.333(43)(121,211); 3.545(34)(040,400); 3.278(77)(330,231,321); 2.9656(88)(141,002,411); 2.5485(93)(051,222,501); 1.873(39)(multiple). Bobmeyerite has the same structural framework as cerchiaraite and ashburtonite. In the structure, which refined to $R_1 = 0.079$ for 1057 reflections with $F > 4\sigma F$, SiO_4 tetrahedra share corners to form four-membered Si_4O_{12} rings centred on the c axis. The rings are linked by chains of edge-sharing AlO_6 octahedra running parallel to [001]. The framework thereby created contains large channels, running parallel to [001]. The Cl site is centred on the c axis alternating along [001] with the Si_4O_{12} rings. Two non-equivalent Pb atoms are positioned around the periphery of the channels. Both are eleven-coordinate, bonding to the Cl atom on the c axis, to eight O atoms in the framework and to two O (H_2O) sites in the channel. The Pb atoms are off-centre in these coordinations, as is typical of Pb^{2+} with stereo-active lone-electron pairs. A $(S,Si,Cr)O_4$ group is presumed to be disordered in the channel. The name honours Robert (Bob) Owen Meyer, one of the discoverers of the new mineral.

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Keywords: bobmeyerite, cerchiaraite, ashburtonite, new mineral, crystal structure, IR spectroscopy, electron microprobe analysis, cyclosilicate, Pb^{2+} $6s^2$ lone-electron pair, Mammoth–Saint Anthony mine, Tiger, Arizona.

Introduction

Bobmeyerite is the tenth new mineral species to be described from the famous Mammoth–Saint Anthony mine at Tiger, Arizona, USA. This mine, which was worked intermittently for baryte, fluorite and ores of gold, lead, molybdenum, silver, tungsten, vanadium and zinc from 1893 to 1953, has yielded a remarkable suite of supergene minerals (Bideaux, 1980). The new mineral, described herein, is almost certainly identical to the phase reported by Bideaux (1980) as an unknown lead silicate occurring in tapered colourless transparent needles, and to the phase listed by Smith and Nickel (2007) as invalid unnamed mineral UM1980-//-SiO:Pb. The other minerals first described from the mine are bideauxite, creaseyite, georgerobinsonite, macquartite, mammothite, murdochite, pinalite, wherryite and yedlinite.

The name honours Robert (Bob) Owen Meyer (b. 1956) of Maple Valley, Washington, USA. Mr Meyer acquired his first specimen from the Mammoth–Saint Anthony mine in 1978 and has subsequently spent thousands of hours studying specimens from the deposit. He has submitted many unusual samples for identification, and in 2008 discovered the first North American occurrence of the rare mineral munakataite on a specimen from the mine. Interestingly, Mr Meyer noticed the new mineral, described herein, on the first specimen he acquired in 1978. It was submitted for identification in the late 1980s, and although it was recognized as a probable new species at the time, the difficulty of working with the thin needles prevented its characterization. More recently, Bob and fellow collectors Joe Ruiz and Brent Thorne reawakened interest in the mineral and submitted new specimens for analysis. These have finally allowed it to be characterized as a new species.

The new mineral and name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2012-019). As no single specimen provided all of the data for the description, there is no specimen that qualifies as the holotype. However, three cotype specimens are housed in the collections of Mineral Sciences Department, Natural History Museum of Los Angeles County (900 Exposition Boulevard, Los Angeles, California 90007, USA), catalogue numbers 63824, 63825 and 63826.

Occurrence

Bobmeyerite occurs at the Mammoth–Saint Anthony mine, Tiger, Pinal County, Arizona, USA (32º42′23″N, 110º40′59″W). The most complete description of the mineralogy of this deposit is provided by Bideaux (1980). The new mineral occurs in an oxidation zone assemblage that includes atacamite, caledonite, cerussite, connellite, diaboleite, fluorite, georgerobinsonite, hematite, leadhillite, matlockite, murdochite, phosgenite, pinalite, quartz, wulfenite and yedlinite. The mode of occurrence is consistent with the "anomalous sequence" of mineralization discussed by Bideaux (1980) and attributed to progressive alteration and crystallization in a closed system.

Physical and optical properties

Bobmeyerite occurs as colourless to white or cream-coloured needles which are elongated on [001] and taper to sharp points. No forms could be measured optically, but SEM images suggest relatively equal development of {100} and {010}. The needles occur in jumbled aggregates and Bideaux (1980) noted that some of them "wander across cavities and look astonishingly like woolly caterpillars" (Fig. 1). Crystals are up to about 300 μm in length and generally less than 2 μm in diameter (Fig. 2). No twinning was observed.

The crystals have a white streak, are transparent to translucent and have a vitreous lustre. They do not fluoresce in either long-wave or short-wave ultraviolet light. The hardness and fracture could not be determined because of the very small thickness of the needles. The tenacity is brittle and no cleavage was observed. The density could not be measured; it is greater than those of available high-density liquids and there is insufficient material for a physical determination. The calculated density is 4.381 g cm^{-3}, based on

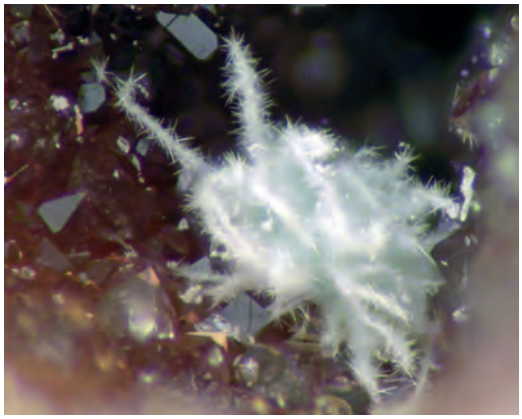

FIG. 1. Bobmeyerite 'woolly caterpillars' on quartz. The field of view is 1.2 mm. This is a composite stacked image taken by Bob Meyer from a specimen is his collection.

the empirical formula and the unit-cell parameters determined by single-crystal X-ray diffraction. Bobmeyerite dissolves very slowly in concentrated HCl; it is insoluble and unreactive in concentrated H_2SO_4 and 70% HNO_3.

The optical properties were measured in white light. Bobmeyerite is biaxial negative, with $\alpha \approx \beta = 1.759(2)$ and $\gamma = 1.756(2)$. The small size of the fibres precluded conoscopic observation, and therefore the 2V could not be determined, but it is expected to be very small. The optical orientation is X = **c**; Y or Z = **a** or **b**. Bobmeyerite is not pleochroic.

Infrared spectroscopy

For analysis by Fourier transform infrared (FTIR) spectroscopy, a sample was positioned on a Spectra-Tech low-pressure diamond microsample cell and analysed using a Bruker Optics Hyperion 2000 microscope interfaced to a Tensor 27 spectrometer. The spectrum was acquired in the 4000 to 430 cm^{-1} range by co-adding 150 scans (Fig. 3). The absorption at 3386 cm^{-1} can be assigned to OH and that at 1649 cm^{-1} to H_2O. The absorption peaks in the 1200–430 cm^{-1} region are similar to those in the spectrum of ashburtonite and include contributions from both the SiO_4 tetrahedra and the four-member silicate ring. It was not possible to verify or disprove the presence of SO_4 or CrO_4 groups on the basis of the FTIR data, but CO_3 is absent as there are no characteristic CO_3 absorption bands.

Chemical composition

Chemical analyses were carried out on a JEOL 8200 electron microprobe in wavelength-dispersive spectrometry (WDS) mode at the Division of Geological and Planetary Sciences, California Institute of Technology, operating at 10 kV, 5 nA with a focussed beam. Data were processed with the *CITZAF* correction procedure. The

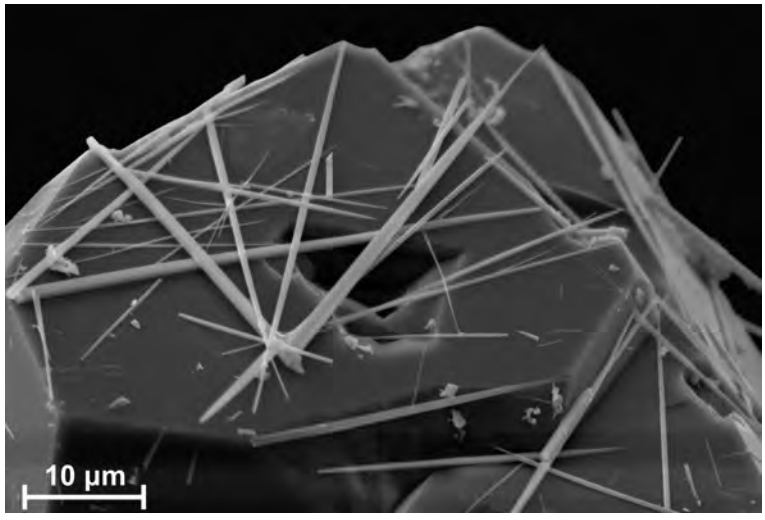

FIG. 2. Scanning electron microscope image of bobmeyerite needles on quartz.

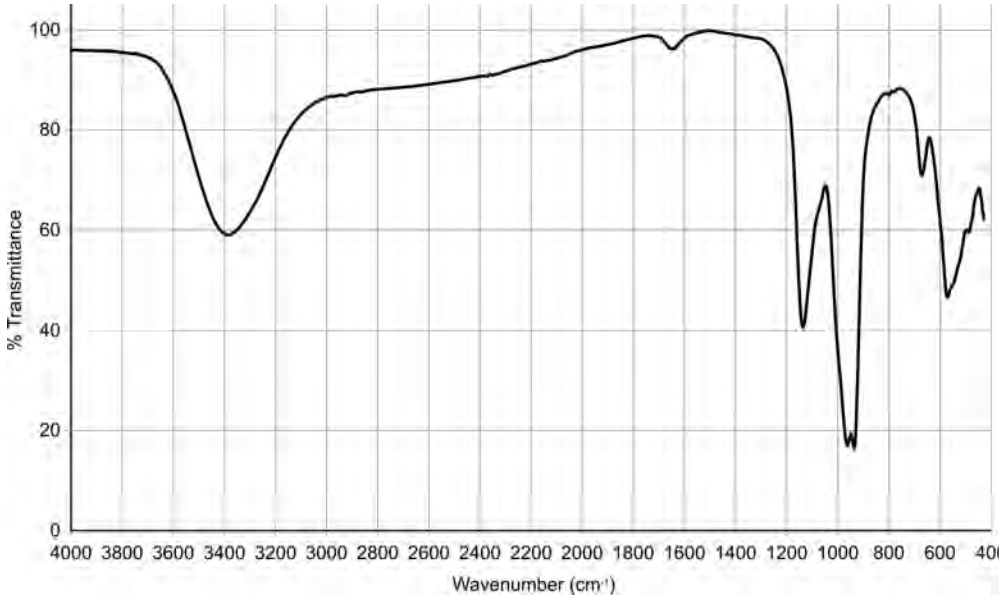

FIG. 3. The FTIR spectrum of bobmeyerite.

standards used were galena (for Pb), synthetic anorthite (for Al, Si and Ca), synthetic Cr_2O_3 (for Cr), anhydrite (for S), synthetic fluorophlogopite (for F) and sodalite (for Cl); Mg, V and Fe were sought, but not detected. There was insufficient material for CHN analyses, and therefore H_2O was calculated on the basis of Al + Cu = 4, charge balance and 27 total anions (O + Cl + F) p.f.u., based on structural considerations (see below); the presence of H_2O and OH and the absence of CO_3 were confirmed by FTIR spectroscopy.

Bobmeyerite was challenging to analyse due to the small size and very limited thickness of the acicular crystals. The largest grain found was only 2 μm across, and most grains were 1 μm or less. Flat areas on the two largest crystals appeared to

TABLE 1. Analytical data for bobmeyerite.

	– Corrected but not normalized –					Normalized					
	1-1	1-2	2-1	2-2	2-3	1-1	1-2	2-1	2-2	2-3	Mean
CaO	0.16	0.14	0.12	0.15	0.13	0.17	0.13	0.12	0.16	0.13	0.14
PbO	49.40	58.28	53.82	51.96	58.71	53.37	54.42	55.00	54.87	56.48	54.83
CuO	5.61	5.26	4.98	4.05	4.53	6.06	4.91	5.09	4.28	4.36	4.94
Al_2O_3	8.95	11.14	9.43	9.80	10.42	9.67	10.4	9.64	10.35	10.02	10.02
SiO_2	15.58	18.10	16.44	17.05	17.60	16.83	16.9	16.8	18.01	16.93	17.09
SO_3	2.96	2.93	3.03	2.86	3.08	3.20	2.74	3.10	3.02	2.96	3.00
CrO_3	0.41	0.59	1.43	0.80	1.00	0.44	0.55	1.46	0.84	0.96	0.85
F	0.80	0.36	0.75	0.53	0.71	0.86	0.34	0.77	0.56	0.68	0.64
Cl	2.13	1.93	3.10	2.57	2.17	2.30	1.80	3.17	2.71	2.09	2.41
H_2O*	7.39	8.96	5.78	5.72	6.39	7.98	8.37	5.91	6.04	6.15	6.89
O=F,Cl	−0.82	−0.59	−1.02	−0.80	−0.79	−0.89	−0.55	−1.04	−0.84	−0.76	−0.81
Total	92.57	107.10	97.86	94.69	103.95	99.99	100.01	100.02	100.00	100.00	100.00

* The H_2O values are based upon the structure, with 27 total anions and Al + Cu = 4.
Means are calculated from the normalized data.

TABLE 2. Powder X-ray data for bobmeyerite.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	*hkl*
35	10.051	9.9718	77	110
6	7.104	7.1285	4	020
		6.9762	5	200
7	6.367	6.3480	6	120
		6.2663	5	210
54	5.474	5.4516	33	011
		5.4341	30	101
35	5.011	4.9859	54	220
5	4.516	4.4986	7	130
43	4.333	4.3216	22	121
		4.2956	21	211
6	3.921	3.9276	5	230
		3.8951	6	320
7	3.680	3.7010	3	031
		3.6525	5	301
34	3.545	3.5773	4	131
		3.5643	18	040
		3.5382	3	311
		3.4881	20	400
77	3.278	3.3239	11	330
		3.2694	49	231
		3.2506	37	321
88	2.966	3.1740	5	240
		2.9804	37	141
		2.9500	31	002
		2.9382	44	411
7	2.831	2.8288	4	112
9	2.747	2.7937	6	150
		2.7385	5	510
		2.7258	3	022
		2.7171	3	202
100	2.549	2.5673	24	051
		2.5389	53	222
		2.5249	3	151
		2.5226	19	501
6	2.498	2.4930	18	440
5	2.430	2.4309	5	350
22	2.265	2.2726	8	042
		2.2525	9	402
23	2.218	2.2108	4	620
		2.2064	15	332
28	2.072	2.0676	17	451
		2.0591	12	541
20	2.001	2.0284	5	152
		2.0070	4	512
		1.9944	5	550
		1.9918	3	361
4	1.958	1.9690	6	631
		1.9482	3	013
		1.9474	3	103
39	1.873	1.9072	3	171
		1.9041	6	442
		1.8786	3	123
		1.8764	3	213
		1.8760	3	352
		1.8720	3	711
		1.8657	6	370
		1.8633	3	461
		1.8559	13	271
25	1.837	1.8494	3	641
		1.8381	5	730
		1.8254	11	721
27	1.7693	1.7887	6	262
		1.7691	9	622
		1.7675	3	452
		1.7621	4	542
		1.7585	8	233
		1.7556	6	323
7	1.7100	1.7090	6	143
		1.7009	8	413
11	1.6572	1.6641	3	172
		1.6522	11	552
16	1.6209	1.6189	6	053
		1.6075	5	503
4	1.5737	1.5768	3	372
		1.5600	3	732
8	1.5314	1.5299	2	091
		1.5208	3	191
8	1.5033	1.5164	2	182
		1.5013	1	802
		1.4994	2	901
20	1.4767	1.4830	2	671
		1.4750	8	004
		1.4685	5	453
		1.4654	3	543
4	1.4465	1.4494	2	382
		1.4427	2	851
		1.4405	1	363
6	1.4320	1.4319	2	633
5	1.4173	1.4245	3	770
		1.4144	4	224
17	1.3909	1.4011	4	491
		1.3887	3	192
		1.3865	5	273
		1.3821	3	941
25	1.3704	1.3755	1	681
		1.3737	4	723
		1.3677	1	861
		1.3660	3	912
		1.3631	1	3·10·0
		1.3629	2	044
		1.3585	3	404

Calculated lines with relative intensities of less than 5 are not listed unless they correspond to observed lines.

be relatively stable in the electron beam, giving analytical totals that did not decrease as a function of time; however, the totals range from 92.57 to 107.10 wt.% when calculated H_2O is included. This is attributed to a combination of dehydration under vacuum (which would produce high values) and the limited thickness of the grains (which would produce low values). Regardless of the variability in the totals, generally consistent elemental ratios were obtained. Original and normalized analyses are listed in Table 1.

The empirical formula for bobmeyerite (based on 27 anions) is $Pb_{3.80}Ca_{0.04}Al_{3.04}Cu^{2+}_{0.96}Cr^{3+}_{0.13}Si_{4.40}S_{0.58}O_{24.43}Cl_{1.05}F_{0.52}H_{11.83}$. The simplified formula recast using information from the structural analysis is $(Pb,Ca)_4(Al,Cu)_4(Si_4O_{12})[(S,Si,Cr)O_4][(OH),F]_7Cl(H_2O)_3$. The simplified endmember formula $Pb_4Al_4(Si_4O_{12})(SO_4)(OH)_7Cl(H_2O)_3$ has a charge of +2, and we therefore propose that the charge-balanced ideal formula should be $Pb_4(Al_3Cu)(Si_4O_{12})(S_{0.5}Si_{0.5}O_4)(OH)_7Cl(H_2O)_3$, which requires PbO 56.50, Al_2O_3 9.68, CuO 5.03, SiO_2 17.11, SO_3 2.53, Cl 2.24, H_2O 7.41, O=Cl −0.51; total 99.99 wt.%.

The Gladstone–Dale compatibility index, $1 - (K_P/K_C)$, based on the calculated density and empirical formula, is 0.007, which is superior according to the classification of Mandarino (1981).

X-ray crystallography and structure refinement

The powder X-ray diffraction study was carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with monochromatic Mo$K\alpha$ radiation. The observed

TABLE 3. Data collection and structure refinement for bobmeyerite.

Diffractometer	Huber 4-circle diffractometer with Bruker 6000 SMART CCD detector
X-ray radiation wavelength	0.40651 Å
Temperature	293(2) K
Structural formula	$Pb_4(Al_{3.28}Cu_{0.72})(Si_4O_{12})(OH)_8Cl[(H_2O)_{1.73}(OH)_{2.27}]$
Space group	*Pnnm*
Unit-cell dimensions	a = 13.969(9) Å
	b = 14.243(10) Å
	c = 5.893(4) Å
V	1172.4(1.4) Å^3
Z	2
Density (for above formula)	4.274 g cm^{-3}
Absorption coefficient	16.248 mm^{-1}
F(000)	1340.5
Crystal size	80 × 2 × 2 μm
θ range	1.64 to 15.66°
Index ranges	$-15 \leqslant h \leqslant 18$, $-14 \leqslant k \leqslant 18$, $-7 \leqslant l \leqslant 7$
Refls collected / unique	10,555 / 1552 [R_{int} = 0.12]
Reflections with $F_o > 4\sigma F$	1057
Completeness	98.1%
Refinement method	Full-matrix least-squares on F^2
Parameters refined	99
GoF	1.060
Final R indices [$F_o > 4\sigma F$]	R_1 = 0.0791, wR_2 = 0.1589
R indices (all data)	R_1 = 0.1231, wR_2 = 0.1739
Largest diff. peak / hole	+4.18 / −3.60 e A^{-3}

$R_{int} = \Sigma|F_o^2 - F_o^2(mean)|/\Sigma[F_o^2]$.
GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$.
$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.
$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where a is 0.0552, b is 114.8607 and P is $[2F_c^2 + \text{Max}(F_o^2,0)]/3$.

TABLE 4. Atom coordinates and displacement parameters (Å^2) for bobmeyerite.

	x/*a*	*y*/*b*	*z*/*c*	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb1	0.72313(11)	0.48502(9)	0	0.0312(4)	0.0477(9)	0.0294(6)	0.0163(5)	0	0	−0.0031(6)
Pb2	0.51318(10)	0.71552(10)	0	0.0300(4)	0.0354(7)	0.0381(7)	0.0166(5)	0	0	−0.0036(6)
Al*	0.7684(4)	0.2688(3)	0.7506(8)	0.0226(18)	0.033(3)	0.029(3)	0.006(2)	−0.0006(19)	0.001(2)	0.013(2)
Cu*	0.7684(4)	0.2688(3)	0.7506(8)	0.0226(18)	0.033(3)	0.029(3)	0.006(2)	−0.0006(19)	0.001(2)	0.013(2)
Cl	½	½	0	0.030(3)	0.044(7)	0.031(6)	0.016(5)	0	0	−0.001(5)
Si1	0.5942(6)	0.6270(6)	½	0.0202(18)	0.025(5)	0.028(5)	0.008(4)	0	0	−0.006(4)
Si2	0.6296(6)	0.4081(6)	½	0.0184(18)	0.032(5)	0.016(4)	0.008(4)	0	0	0.008(3)
O1	0.6323(18)	0.5200(15)	½	0.031(5)	0.040(15)	0.023(11)	0.030(12)	0	0	−0.002(11)
O2	0.4787(16)	0.6313(16)	½	0.028(5)	0.030(13)	0.036(13)	0.018(10)	0	0	−0.016(11)
O3	0.6314(11)	0.6780(10)	0.274(2)	0.024(3)	0.041(9)	0.025(7)	0.004(6)	0.000(6)	0.000(6)	−0.017(7)
O4	0.6803(10)	0.3691(10)	0.728(2)	0.021(3)	0.025(8)	0.026(8)	0.013(7)	−0.005(6)	−0.004(6)	−0.002(6)
OH5	0.7036(17)	0.2162(18)	0	0.035(6)	0.035(14)	0.044(14)	0.027(13)	0	0	0.007(12)
OH6	0.7105(17)	0.2051(16)	½	0.034(6)	0.033(13)	0.026(12)	0.042(15)	0	0	0.007(11)
OH7	0.6591(15)	0.8225(15)	0	0.025(5)	0.014(10)	0.030(11)	0.031(12)	0	0	0.008(10)
OH8	0.8258(16)	0.3398(19)	0	0.039(6)	0.017(12)	0.061(17)	0.038(15)	0	0	0.013(12)
OW9	0.630(5)	0.028(5)	0	0.17(3)						
OW10	0.032(6)	0.366(6)	0	0.22(4)						

* Refined site occupancy: Al 0.820(18), Cu 0.180(18).

d-spacings and relative intensities derived by profile fitting using *JADE 9.3* software are listed in Table 2. Unit-cell parameters refined from the powder data using *JADE 9.3* software with whole-pattern fitting are as follows: a = 13.952(3), b = 14.257(3), c = 5.9000(10) Å and V = 1173.6(4) Å^3. These unit-cell parameters were used to determine the calculated *d*-spacings and intensities listed in Table 2.

Single-crystal structure data were obtained at ChemMatCARS, Sector 15, Advanced Photon Source at Argonne National Laboratory, USA. These data were integrated and corrected for Lorentz, polarization and background effects and systematic errors, such as beam decay and absorption, using *SAINTPLUS* and *SADABS* (Bruker, 2005). The structure was solved by direct methods and refined using *SHELXTL* (Sheldrick, 2008).

In the final stages of structure refinement, the largest residual electron densities were in the immediate vicinities of the Pb sites. Attempts to split the Pb atoms into multiple partially occupied sites were marginally effective, reducing R_1 to about 0.074, but they confirmed that the vast majority of the Pb occupancies (~0.92) remained at the original unsplit sites. An attempt was also made to refine the occupancies of the unsplit Pb sites, but this yielded only slightly less than full occupancies and left the R_1 index unaffected. Consequently, the final structure refinement was based on unsplit, fully occupied Pb sites. It is probable that the F reported in the chemical analysis is distributed among the OH sites bonded to Al. As the OH sites account for 8 O + F p.f.u., of which there is only 0.52 F p.f.u and the scattering powers of O and F are not very different, no attempt was made to refine the occupancies of the OH sites.

Details of the data collection and the final structure refinement are provided in Table 3. The final atom coordinates and displacement parameters are listed in Table 4. Selected interatomic distances are listed in Table 5. A bond-valence analysis is provided in Table 6. A list of observed and calculated structure factors has been deposited with *Mineralogical Magazine* and can be downloaded from http://www.minersoc.org/pages/e_journals/dep_mat_mm.html.

Description of the structure

Bobmeyerite has the same structural framework as cerchiaraite (Basso *et al*., 2000; Kampf *et al*., 2013) and ashburtonite (Grice *et al*., 1991), although it is orthorhombic, rather than tetragonal (Fig. 4). In the structure, SiO_4 tetrahedra share corners to form four-membered Si_4O_{12} rings centred on the c axis. The rings are linked by chains of edge-sharing AlO_6 octahedra which also run parallel to [001]. The framework thereby created contains large channels, which run parallel to [001]. The Cl site is centred on the c axis and alternates along [001] with the Si_4O_{12} rings. Two non-equivalent Pb atoms are located around the periphery of the channels. Both are eleven-coordinate, bonding to the Cl atom on the c axis, to eight O atoms in the framework and to two O sites in the channel. They are off-centre in these coordinations, as is typical of Pb^{2+} with stereo-active lone-electron pairs.

A few remarks regarding the channel constituents are warranted. The channel O sites (OW9 and OW10) have very large isotropic thermal parameters, suggesting that they are loosely bonded to the Pb atoms (as was reported for the CO_3 group in ashburtonite). The OW9 and OW10 bonds to the Pb atoms have bond-valence sums (Table 6) that are consistent with H_2O groups; however, these sites probably also participate to some extent in bonds to S, Si and Cr in the channel. The S, Cr and excess Si determined by EMPA, $(S_{0.58}Si_{0.40}Cr^{3+}_{0.13})_{\Sigma 1.11}$, must be accommodated in the channel, presumably in tetrahedral coordination to O. We were unable to resolve a tetrahedral cation site in the channel; however, the considerable residual electron density leaves a good deal of latitude for accommodating additional constituents.

Resolving the formula of bobmeyerite

If H_2O cannot be directly determined, it is commonly calculated based upon the amount indicated by the crystal structure analysis and, in particular, by the number of O atoms. For a structure that includes unresolved disordered channel sites, such as that of bobmeyerite, it is not possible to rigorously define the number of O atoms based upon refined structural sites. Channel volume and packing considerations can provide a theoretical upper limit, but if a Pb^{2+} cation with stereo-active lone-electron pairs is present, calculations based on sphere packing become less reliable. In bobmeyerite, the channel constituents are certainly not very efficiently packed.

The two refined channel sites can reasonably be assigned to O atoms of H_2O groups, providing a total of 25 anions (O + Cl + F) p.f.u., but

TABLE 5. Selected bond distances (Å) in bobmeyerite.

Pb1–O4 (×2)	2.376(14)	Pb2–O3 (×2)	2.369(15)	Al–OH5	1.881(17)	Si1–O3 (×2)	1.606(14)
Pb1–OH8	2.52(2)	Pb2–OH7	2.55(2)	Al–O4	1.890(15)	Si1–O1	1.61(2)
Pb1–Cl	3.124(3)	Pb2–Cl	3.075(3)	Al–O3	1.910(14)	Si1–O2	1.61(2)
Pb1–O1 (×2)	3.247(10)	Pb2–OH5	3.18(2)	Al–OH6	1.912(16)	**<Si–O>**	**1.612**
Pb1–OH6	3.27(2)	Pb2–O2 (×2)	3.217(9)	Al–OH7	1.947(14)		
Pb1–O3 (×2)	3.434(15)	Pb2–O4 (×2)	3.364(15)	Al–OH8	1.956(19)	Si2–O1	1.59(2)
Pb1–OW9 (×2)	3.64(4)	Pb2–OW10 (×2)	3.70(5)	**<Al–O>**	**1.916**	Si2–O2	1.61(2)
<Pb–φ>	**3.119**	**<Pb–φ>**	**3.100**			Si2–O4 (×2)	1.619(15)
						<Si–O>	1.610

TABLE 6. Bond-valence analysis for bobmeyerite. Values are expressed in valence units.

	O1	O2	O3	O4	OH5	OH6	OH7	OH8	OW9	OW10	Cl	Σ
Pb1	0.05 ×2↓→		0.03 ×2→	0.49 ×2→		0.04		0.33	0.02 ×2↓→		0.20 ×2↓	1.75
Pb2		0.05 ×2↓→	0.50 ×2→	0.03 ×2→	0.06		0.31			0.01 ×2↓→	0.23 ×2↓	1.78
Al			0.50	0.53	0.54 ×2↓	0.50 ×2↓	0.46 ×2↓	0.44 ×2↓				2.98
Si1	1.01	1.04	1.05 ×2→									4.15
Si2	1.04	1.04		1.01 ×2→								4.10
Σ	2.15	2.18	2.08	2.06	1.14	1.04	1.23	1.21	0.04	0.02	0.86	

Bond valence for the Al site is based on the refined occupancy indicated in Table 4. Multiplicity is indicated by ×↓→. All bond strengths are from Brown and Altermatt (1985).

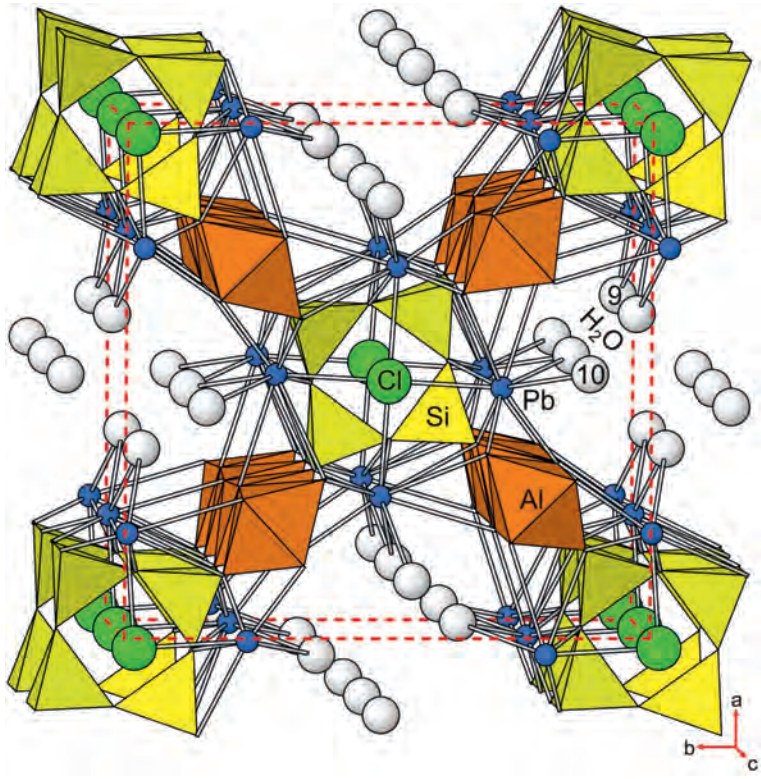

FIG. 4. The structure of bobmeyerite canted slightly from [001]; Pb–φ bonds are shown as thin rods. The outline of the unit cell is shown by a dashed red line.

considerable widely dispersed residual electron density remains in the channel. Some of this electron density probably corresponds to approximately one cation, $(S_{0.58}Si_{0.40}Cr^{3+}_{0.13})_{\Sigma 1.11}$, p.f.u. tetrahedrally coordinated to O atoms. If this tetrahedral group is linked in a similar manner to the SiO_4 group in the channel of the cerchiaraite structure, three of its corners would be formed by O atoms bonded to three different Pb atoms and one would be an OH site (OH5, OH6, OH7 and/or OH8) of the Al octahedron. Adjacent OW sites cannot participate in the same tetrahedral coordination because no OW–OW pair is closer than 3.59 Å; therefore, there must be additional disordered O sites in the channel. As the tetrahedral group is essentially ¼ occupied and disordered in the channel, it is not surprising that it remains unresolved in the structure refinement.

Assuming that statistically ¼ of each OW participates in a $(S,Si,Cr)O_4$ group, the OW9 and OW10 sites account for a total of three H_2O groups p.f.u. in the channel. Combining that with one $(S,Si,Cr)O_4$ group p.f.u. requires that the formula be based upon 27 anions. For comparison, the formula of cerchiaraite is based on 27 anions (Kampf *et al.*, 2013) and that of ashburtonite is based on 29. Using 27 anions, the simplified structural formula for bobmeyerite is $(Pb,Ca)_4(Al,Cu)_4(Si_4O_{12})[(S,Si,Cr)O_4][(OH),F]_7Cl(H_2O)_3$. The endmember formula $Pb_4Al_4(Si_4O_{12})(SO_4)(OH)_7Cl(H_2O)_3$ has a net charge of +2; replacing Al_4 by Al_3Cu and SO_4 by $S_{0.5}Si_{0.5}O_4$ yields the charge-balanced ideal formula $Pb_4(Al_3Cu)(Si_4O_{12})(S_{0.5}Si_{0.5}O_4)(OH)_7Cl(H_2O)_3$.

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Cu OH7 Al 98.7(10) 8_765 3_655 ?
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Cu OH7 Pb2 100.4(8) 8_765 . ?
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Cu OH7 Pb1 57.8(4) 8_765 3_655 ?
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Cu OH7 Pb1 124.0(8) 3_655 3_655 ?
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Pb2 OH7 Pb1 131.3(3) . 3_655 ?
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Pb2 OH7 Pb1 131.3(3) . 3_654 ?
Pb1 OH7 Pb1 92.1(5) 3_655 3_654 ?
Cu OH8 Al 0.0(4) 1_554 1_554 ?
Cu OH8 Cu 97.4(12) 1_554 6_556 ?
Al OH8 Cu 97.4(12) 1_554 6_556 ?
Cu OH8 Al 97.4(12) 1_554 6_556 ?
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Al OH8 Pb1 101.0(8) 6_556 . ?
Cu OH8 Pb2 122.7(10) 1_554 3_645 ?
Al OH8 Pb2 122.7(10) 1_554 3_645 ?
Cu OH8 Pb2 57.5(4) 6_556 3_645 ?
Al OH8 Pb2 57.5(4) 6_556 3_645 ?
Pb1 OH8 Pb2 131.8(4) . 3_645 ?
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Pb1 OH8 Pb2 131.8(4) . 3_644 ?
Pb2 OH8 Pb2 91.7(5) 3_645 3_644 ?
Pb1 OW9 Pb1 108.1(18) 3_645 3_644 ?
Pb2 OW10 Pb2 106(2) 3_544 3_545 ?
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Pb2 OW10 Pb1 116.7(14) 3_545 5_665 ?

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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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