

# Dervillite, $\text{Ag}_2\text{AsS}_2$ , from Lengenbach quarry, Binn valley, Switzerland: occurrence and crystal structure

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## ABSTRACT

Dervillite,  $\text{As}_2\text{AsS}_2$ , has been found in a sample from the Lengenbach quarry in the Binn Valley, Valais, Switzerland. It occurs as very rare crystals up to 200  $\mu\text{m}$  across on jordanite. Dervillite is opaque with a metallic lustre and shows a dark brown streak. The structure is monoclinic, space group  $Pc$ , with  $a = 9.6155(7)$ ,  $b = 12.9331(8)$ ,  $c = 6.8616(5)$  Å,  $\beta = 99.352(8)^\circ$ ,  $V = 842.0(1)$  Å<sup>3</sup> and  $Z = 8$ . In the crystal structure [ $R_1 = 0.060$  for 2370 reflections with  $I > 2\sigma(I)$ ], silver adopts various coordinations extending from quasi linear to quasi tetrahedral whereas arsenic forms very peculiar crystal-chemical environments, such as  $\text{As}(\text{S}_2\text{As})$  and  $\text{As}(\text{S}_2\text{AsAg})$ . Such metalloid–metalloid or metal–metalloid bonds account for the apparent charge imbalance observed in the chemical formula.

**KEYWORDS:** dervillite, silver, Lengenbach, Switzerland.

## Introduction

DERVILLITE was described first by Weil (1941) as a natural compound of lead, sulfur and antimony, and possibly also bismuth. A reinvestigation of the original sample by Bari *et al.* (1983) proved that the chemical data given by Weil (1941) were erroneous, because they were based on chemical tests on material that was apparently not extracted from the dervillite crystals. Unfortunately, given wartime conditions, the study could not be completed. By means of X-ray single-crystal precession photographs and an X-ray powder diffraction study of the holotype, Bari *et al.* (1983) found that dervillite is monoclinic, space group  $P2/a$ , with  $a = 6.833$ ,  $b = 12.932$ ,  $c = 9.638$  Å,  $\beta = 99.33^\circ$ ,  $V = 1715.9(7)$  Å<sup>3</sup> and  $Z = 8$ . New electron microprobe analyses indicated the presence of only Ag, As and S, giving rise to the  $\text{Ag}_2\text{AsS}_2$  chemical formula. However, a full

structural study was never carried out and the dervillite structure remains unknown.

In the course of a research project dealing with Ag-rich minerals from the Lengenbach quarry, Binn Valley, Canton Valais, Switzerland (Nestola *et al.*, 2010; Bindi *et al.*, 2010a, 2012a,b, 2013; Guastoni *et al.*, 2012) we discovered a dervillite crystal (Fig. 1) in a sample coming from the so-

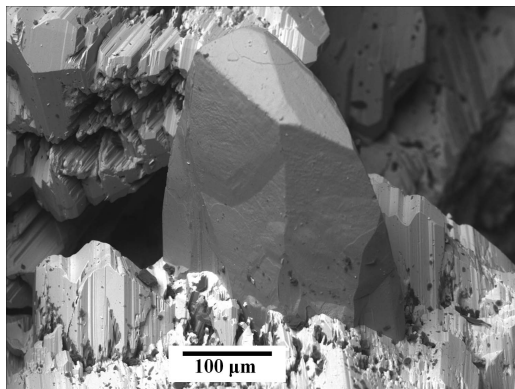


FIG. 1. SEM-BSE image of dervillite on jordanite.

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called zone 0 (Graeser *et al.*, 2008), collected in 1998. This zone is particularly enriched in jordanite, galena and Ag-rich sulfosalts such as marrite, quadratite, proustite and xantoconite.

Here we report the description of the new occurrence of dervillite, together with the determination of its crystal structure.

A chemical analysis using energy dispersive spectrometry (EDS) performed using a SEM JEOL-5610 LV at the Museum of Natural History of Milan showed the presence of Ag, As and S only, with stoichiometry nearly identical to  $\text{Ag}_2\text{AsS}_2$ .

### Occurrence and chemical data

Dervillite occurs as very rare, well developed crystals on jordanite (Fig. 1). The mineral does not show any inclusions of, or intergrowths with, other minerals. The maximum grain size of dervillite recovered in the sample studied is  $\sim 200 \mu\text{m}$ . It is dark grey in colour and shows a dark-brown streak. The mineral is opaque in transmitted light and exhibits a metallic lustre. No cleavage is observed and the fracture is uneven.

### X-ray crystallography and crystal-structure determination

The same crystal fragment ( $85 \mu\text{m} \times 170 \mu\text{m} \times 180 \mu\text{m}$ ) used to obtain the EDS chemical data was selected for the X-ray single-crystal diffraction study that was done using a STOE-STADI IV CCD single-crystal diffractometer (Table 1). The mineral was found to be monoclinic, with  $a = 9.6155(7)$ ,  $b = 12.9331(8)$ ,  $c = 6.8616(5) \text{ \AA}$ ,  $\beta = 99.352(8)^\circ$ ,  $V = 842.0(1) \text{ \AA}^3$  and  $Z = 8$  [we preferred to adopt  $a$  and  $c$

TABLE 1. Crystallographic data and refinement parameters for dervillite.

<b>Crystal data</b>	
Ideal formula	$\text{Ag}_2\text{AsS}_2$
Crystal system	Monoclinic
Space group	$Pc$ (#7)
Unit-cell parameters ( $\text{Å}$ , $^\circ$ )	9.6155(7) 12.9331(8) 6.8616(5), 99.352(8)
Unit-cell volume ( $\text{Å}^3$ )	842.0(1)
$Z$	8
Crystal size (mm)	$0.085 \times 0.170 \times 0.180$
<b>Data collection</b>	
Diffractometer	STOE-STADI IV CCD
Temperature (K)	298(3)
Radiation, wavelength ( $\text{Å}$ )	$\text{MoK}\alpha$ , 0.71073
$2\theta$ max for data collection ( $^\circ$ )	75.02
Crystal-detector dist. (mm)	50
$h, k, l$ ranges	$-15-14, -20-20, -11-11$
Axis, frames, width ( $^\circ$ ), time per frame (s)	$\omega$ , 503, 1.00, 20
Total reflections collected	13927
Unique reflections ( $R_{\text{int}}$ )	3788 (0.067)
Unique reflections $I > 2\sigma(I)$	2370
Data completeness to $\theta_{\text{max}}$ (%)	99.1
Absorption correction method	X-RED and X-SHAPE
<b>Structure refinement</b>	
Refinement method	Full-matrix least-squares on $F^2$
Data/restraints/parameters	2370/0/182
$R_1$ [ $I > 2\sigma(I)$ ], $wR_2$ [ $I > 2\sigma(I)$ ]	0.0599, 0.1424
$R_1$ all, $wR_2$ all	0.0884, 0.1592
Goodness-of-fit on $F^2$	0.888
Largest diff. peak and hole ( $\text{e}^-/\text{Å}^3$ )	3.73, -2.42

$$R_{\text{int}} = (n/n - 1)^{1/2} [F_o^2 - F_o(\text{mean})^2] / \Sigma F_o^2$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|; wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2};$$

Goof =  $\{ \Sigma [w(F_o^2 - F_c^2)^2] / (n - p) \}^{1/2}$ . Where  $n$  is the number of reflections and  $p$  is the number of refined parameters.

TABLE 2. Atoms, fractional atom coordinates ( $\text{\AA}$ ) and atomic displacement parameters ( $\text{\AA}^2$ ) for derwillite.

Atom	$x/a$	$y/b$	$z/c$	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$	$U_{\text{iso}}$
Ag1	0.2371(2)	0.5959(1)	0.4229(2)	0.051(1)	0.0282(8)	0.0254(7)	-0.0029(6)	0.0049(7)	-0.0037(7)	0.0350(4)
Ag2	0.0416(2)	0.9139(2)	0.7262(3)	0.052(1)	0.044(1)	0.0353(9)	0.0075(7)	-0.0025(8)	0.0149(8)	0.0449(5)
Ag3	0.6931(2)	0.9071(1)	0.1224(2)	0.0372(9)	0.0283(7)	0.0284(8)	0.0014(6)	0.0012(7)	-0.0030(6)	0.0318(4)
Ag4	0.3575(2)	0.8929(1)	0.6293(3)	0.046(1)	0.0234(7)	0.0425(9)	0.0062(7)	0.0145(8)	-0.0062(7)	0.0366(4)
Ag5	0.5650(2)	0.6059(1)	0.8956(3)	0.043(1)	0.0251(7)	0.045(1)	0.0067(7)	0.0152(8)	-0.0036(7)	0.0367(4)
Ag6	0.9615(2)	0.7898(2)	0.3072(3)	0.0360(9)	0.068(1)	0.057(1)	0.027(1)	0.0108(9)	-0.013(1)	0.0531(6)
Ag7	0.8387(4)	0.4927(2)	0.6518(4)	0.109(3)	0.072(2)	0.068(2)	0.048(1)	-0.004(2)	-0.019(2)	0.085(1)
Ag8	0.9610(3)	0.6868(2)	0.8480(5)	0.031(1)	0.073(2)	0.113(2)	0.016(2)	0.008(1)	0.021(1)	0.0728(8)
As1	0.3125(2)	0.6854(1)	0.9386(2)	0.0161(8)	0.0131(7)	0.0189(8)	0.0000(5)	0.0037(6)	0.0021(6)	0.0160(3)
As2	0.6178(2)	0.6817(1)	0.3513(2)	0.0194(9)	0.0211(8)	0.0131(7)	-0.0003(6)	0.0020(6)	-0.0037(6)	0.0179(3)
As3	0.3096(2)	0.8309(1)	0.1799(2)	0.0204(8)	0.0183(7)	0.0126(7)	-0.0008(5)	0.0027(6)	-0.0029(6)	0.0171(3)
As4	0.6260(2)	0.8216(1)	0.6035(2)	0.0158(8)	0.0159(7)	0.0169(8)	0.0020(6)	0.0039(6)	0.0012(6)	0.0160(3)
S1	0.1530(5)	0.5813(3)	0.0500(7)	0.024(2)	0.014(2)	0.018(2)	0.003(1)	0.003(2)	-0.002(1)	0.0185(8)
S2	0.7918(5)	0.9187(3)	0.4999(6)	0.021(2)	0.017(2)	0.018(2)	0.001(1)	0.006(2)	-0.003(1)	0.0185(8)
S3	0.1924(5)	0.7455(3)	0.6573(6)	0.024(2)	0.019(2)	0.015(2)	-0.002(1)	0.003(2)	0.003(2)	0.0193(8)
S4	0.7333(6)	0.7506(3)	0.8916(6)	0.033(3)	0.022(2)	0.011(2)	-0.001(1)	0.001(2)	0.004(2)	0.0221(9)
S5	0.8474(5)	0.6291(3)	0.4149(7)	0.020(2)	0.020(2)	0.021(2)	0.001(2)	0.006(2)	-0.001(1)	0.0199(8)
S6	0.5142(5)	0.5672(3)	0.5224(7)	0.021(2)	0.018(2)	0.029(2)	-0.003(2)	0.010(2)	-0.006(2)	0.0221(9)
S7	0.0916(5)	0.8957(4)	0.1043(7)	0.017(2)	0.030(2)	0.019(2)	0.004(2)	0.007(1)	-0.002(2)	0.0218(8)
S8	0.4272(5)	0.9360(3)	0.0120(7)	0.022(2)	0.017(2)	0.022(2)	0.001(2)	0.007(2)	-0.006(2)	0.0198(8)

parameters exchanged with respect to those given by Bari *et al.* 1983) – see below]. The analysis of the systematic absences ( $h0l$ :  $l = 2n$  and  $00l$ :  $l = 2n$ ) led to the choice of the space groups  $Pc$  and  $P2/c$ , the latter being the space group proposed by Bari *et al.* (1983) (i.e. non standard  $P2/a$  in their orientation of the unit cell). Although the statistical tests on the distribution of  $|E|$  values ( $|E^2 - 1| = 0.793$ ) indicated the absence of an inversion centre, suggesting the choice of the space group  $Pc$ , the structure was initially solved in the  $P2/c$  space group. A residual  $R_1 = 0.21$  value was quickly achieved. However, the preliminary structural model obtained indicated a large spreading of the silver electron density and a large atomic disorder. The structure model was subsequently optimized and an ordered model was sought, but no improvement in  $R$  could be achieved. At this point, a thorough analysis of the structure (essentially based upon the observation of the very large atomic displacement parameters for particular atoms) suggested that some symmetry element of the  $P2/c$  space group should be removed. The reflection and atomic position data sets were then adapted to the  $Pc$  space group (showing the same systematic extinctions) and the structure refined. After several cycles, an ordered solution with full site occupations was finally determined by carefully removing atoms with low site occupations and/or non-realistic distances with neighbouring atoms and adding significant positions found in the difference Fourier syntheses. The structure could be smoothly refined in  $Pc$  without any damping factor or restrictions by the program *SHELXL* (Sheldrick, 2008). The occupancy of all the sites was left free to vary (Ag vs. □; As vs. □; S vs. □) but all the positions were found to be fully occupied. Neutral scattering curves for Ag, As and S were taken from the *International Tables for X-ray Crystallography* (Ibers and Hamilton, 1974). At the last stage, with anisotropic atomic displacement parameters for all the atoms and no constraints, the residual value settled at  $R_1 = 0.0599$  for 2370 observed reflections [ $2\sigma(I)$  level] and 182 parameters and at  $R_1 = 0.0884$  for all 3788 independent reflections.

It is noteworthy that the acentric structural model we obtained does not show large values in the correlation matrix between pairs of atoms which are equivalent in the centrosymmetric space group  $P2/c$ . To test whether the acentric model is preferred to the centric one we also test the presence of twinning by inversion (twin law:

$[0\bar{1}0 / 0\bar{1}0 / 00\bar{1}]$ ) in the non-centrosymmetric structure refinement. Indeed, as is well known, a centrosymmetric structure that is refined as non-centrosymmetric will show a twin scale factor, equivalent to the Flack parameter in the case of inversion twinning (Flack *et al.*, 2006; Müller *et al.*, 2006), that refines to 50% within analytical uncertainty. We found the racemic twin-component scale factor refined to 0.12(3), consistent with a highly asymmetrical distribution of the enantiomorphic components and indicating the acentric model as the right choice.

Experimental details and  $R$  indices are given in Table 1. Fractional atomic coordinates and atomic displacement parameters are reported in Table 2. Bond distances are given in Table 3.

TABLE 3. Selected bond distances (Å) for dervillite.

Ag1–S1	2.562(5)	Ag7–S5	2.387(5)
Ag1–S3	2.596(5)	Ag7–S5	2.410(5)
Ag1–S1	2.626(5)	<Ag7–S>	2.399
Ag1–S6	2.667(5)		
<Ag1–S>	2.613	Ag8–S4	2.403(6)
		Ag8–S1	2.522(5)
Ag2–S7	2.572(5)	Ag8–S3	2.861(6)
Ag2–S2	2.640(5)	<Ag8–S>	2.595
Ag2–S7	2.669(5)		
Ag2–S3	2.701(5)	As1–S3	2.222(5)
<Ag2–S>	2.646	As1–S1	2.265(5)
		As1–As3	2.510(2)
Ag3–S8	2.573(5)	As1–Ag5	2.696(3)
Ag3–S2	2.614(5)	<As1–M>	2.423
Ag3–S2	2.635(5)		
Ag3–S4	2.638(5)	As2–S6	2.223(5)
<Ag3–S>	2.615	As2–S5	2.283(5)
		As2–As4	2.496(3)
Ag4–S8	2.484(5)	<As2–M>	2.334
Ag4–S3	2.508(5)		
Ag4–S8	2.661(5)	As3–S8	2.208(5)
Ag4–As4	2.774(3)	As3–S7	2.239(5)
<Ag4–M>	2.608	As3–As1	2.510(2)
		<As3–M>	2.319
Ag5–S4	2.478(5)		
Ag5–S6	2.479(5)	As4–S2	2.235(5)
Ag5–S6	2.577(5)	As4–S4	2.270(5)
Ag5–As1	2.696(3)	As4–As2	2.496(3)
<Ag5–M>	2.558	As4–Ag4	2.774(3)
		<As4–M>	2.444
Ag6–S7	2.438(5)		
Ag6–S5	2.516(5)		
Ag6–S2	2.809(5)		
<Ag6–S>	2.588		

Structure factors (Table 4) have been deposited with the Principal Editor of *Mineralogical Magazine* at [http://www.minersoc.org/pages/e\\_journals/dep\\_mat\\_mm.html](http://www.minersoc.org/pages/e_journals/dep_mat_mm.html).

## Results and discussion

In the crystal structure of dervillite (Fig. 2) there are eight Ag positions which adopt various coordinations ranging from quasi linear to quasi tetrahedral (Table 3). In detail, one Ag atom (i.e. Ag7) can be considered to be in linear coordination, with an overall mean Ag–S of 2.40 Å, although the S–Ag–S angle departs slightly from 180° [i.e. 173.0(2)°]. Two Ag atoms (i.e. Ag6 and Ag8) may be considered as three-fold coordinated, with an overall mean Ag–S distance of 2.59 Å, in good agreement with the Ag–S distance found for the Ag(1) position in the crystal structure of stephanite, Ag<sub>5</sub>[S|SbS<sub>3</sub>]

(2.54 Å: Ribár and Nowacki, 1970), that found for the Ag position in the crystal structure of pyrargyrite, Ag<sub>3</sub>[SbS<sub>3</sub>] (2.573 Å: Engel and Nowacki, 1966) and those observed for the different polytypes of pearceite (i.e. 2.56, 2.58 and 2.59 Å for the *-T2ac*, *-T2ac*, and *-M2a2b2c* polytypes, respectively; Bindi *et al.*, 2006, 2007). The last 5 silver atoms (i.e. Ag1, Ag2, Ag3, Ag4 and Ag5) adopt a close-to-tetrahedral coordination. Ag1, Ag2 and Ag3 coordinate four S atoms with an overall mean Ag–S distance of 2.62 Å, which matches that found for the Ag(3) position in the crystal structure of stephanite, Ag<sub>5</sub>[S|SbS<sub>3</sub>] (2.68 Å: Ribár and Nowacki, 1970) and that found for the Ag(3) polyhedron in the crystal structure of billingsleyite (2.643 Å: Bindi *et al.*, 2010*b*). In addition, the value of 2.62 Å for AgS<sub>4</sub> compares reasonably well with the value of 2.66 Å extrapolated from Shannon's (1976) tables. On the other hand, Ag4 and Ag5 coordinate three S

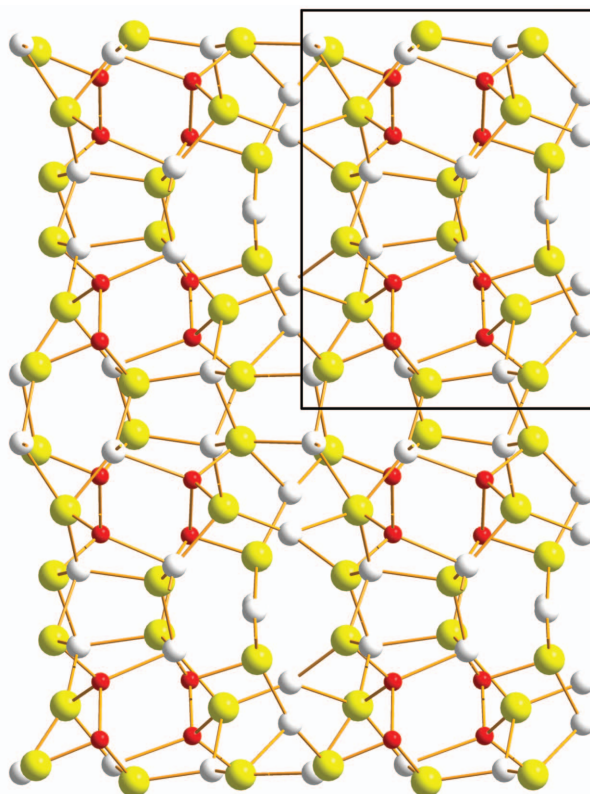


FIG. 2. The crystal structure of dervillite projected down [001]. The vertical direction is the *b* axis. Ag, As and S are given as white, red and yellow spheres, respectively. The unit cell is outlined.

atoms and the tetrahedral configuration is completed by an As atom at a distance of  $\sim 2.7$  Å (Table 3).

The As atoms show very peculiar crystal-chemical environments. If we plot only the As-polyhedra along [010] (Fig. 3), it is evident that the As atoms form columns along the *a* axis. As1 and As4 are in tetrahedral coordination with two S atoms at 2.2–2.3 Å, one As at 2.5 Å and one Ag at  $\sim 2.7$ –2.8 Å. The remaining As2 and As3 atoms exhibit a ‘pyramidal’ coordination with two S and one As. The values observed for the As–As bonds are in keeping with that observed in lautite (Bindi *et al.*, 2008) and those typically observed in As–S molecular compounds (e.g. dimorphite, realgar, uzonite; Bonazzi and Bindi, 2008).

Table 5 shows the X-ray powder pattern calculated using the structural data obtained in this study in comparison with those reported by Bari *et al.* (1983). There is an excellent match between the two patterns except for the first two weak lines (i.e. 5.39 and 3.88 Å) given for the type material.

Finally the chemical formula is considered. Bari *et al.* (1983) proposed to write the formula of dervillite as  $\text{As}_8\text{As}_4\text{S}_8$  (with  $Z = 2$ ) because they speculated on the possible presence of  $\text{As}_4\text{S}_4$  molecular groups coexisting with acanthite-like portions. They hypothesized a unit cell filled by  $8\text{Ag}_2\text{S} + 2\text{As}_4\text{S}_4$ . Such reasoning was driven by the fact that the  $\text{Ag}_2\text{AsS}_2$  formula is not charge-balanced if one considers monovalent silver and trivalent arsenic. However, the structure solution

presented here demonstrates that there is some ‘cation–cation’ bonding (mainly As–As and As–Ag) in the coordination polyhedra of some atoms in dervillite, explaining the apparent charge imbalance observed.

The presence of dimeric  $[\text{As}_2\text{S}_4]^{4-}$  ions with a central As–As bond in dervillite could lead us to write the formula as  $[\text{Ag}^+]_4[\text{As}_2]^{4+}[\text{S}^{2-}]_4$ . However, it is difficult to analyse such polycationic compounds in strict bond-valence terms, as the electronegativity of such elements lies between that of common cations and common anions. The weak Ag–As bonds in dervillite are good examples of the ‘anionic’ behaviour, which could be explained through dative donation of the As lone pair to the closed-shell  $d^{10}$  Ag cations.

Analogies with the dervillite structure can be found in tvalchrelidzeite,  $\text{Hg}_3\text{SbAsS}_3$  (Yang *et al.*, 2007), päakkonenite  $\text{Sb}_2\text{AsS}_2$  (Bonazzi *et al.*, 1995) and chalcotallite  $\text{Tl}_2(\text{Cu},\text{Fe})_6\text{SbS}_4$  (Makovicky *et al.*, 1980). In all of these structures either metalloid–metalloid or metal–metalloid bonds are present, or even entire antimonide portions exist.

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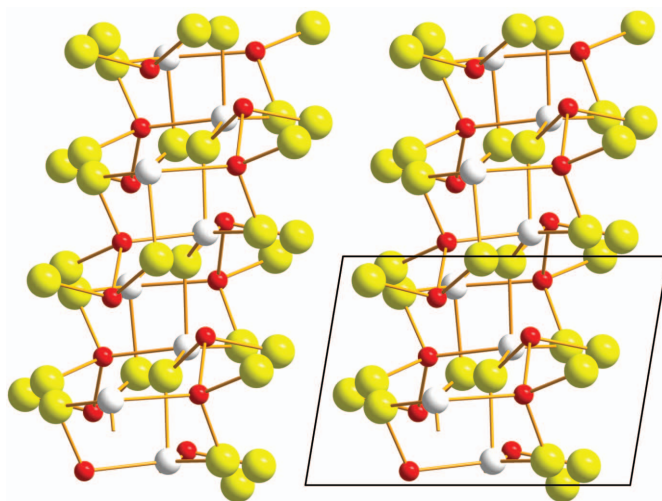


FIG. 3. Portion of the crystal structure of dervillite projected down [010]. Only the coordination polyhedra of the As atoms are depicted. The vertical direction is the *c* axis. Symbols as in Figure 2. The unit cell is outlined.



CRYSTAL STRUCTURE OF DERVILLITE

TABLE 5. X-ray powder diffraction patterns for dervillite.

1			2			1			2		
<i>hkl</i>	<i>d</i> <sub>calc</sub> (Å)	<i>I</i> <sub>calc</sub>	<i>hkl</i>	<i>d</i> <sub>obs</sub> (Å)	<i>I</i> / <i>I</i> <sub>0</sub>	<i>hkl</i>	<i>d</i> <sub>calc</sub> (Å)	<i>I</i> <sub>calc</sub>	<i>hkl</i>	<i>d</i> <sub>obs</sub> (Å)	<i>I</i> / <i>I</i> <sub>0</sub>
100	9.488	5				340	2.2609	5			
110	7.650	6				341	2.2235	5			
—	—	—	111̄	5.39	1	421	2.2182	11			
1̄21	4.3946	5				332	2.1786	8			
121	4.0194	6				302	2.1437	20	213̄, 123̄	2.142	1
—	—	—	130	3.88	1	312	2.1149	15	402	2.114	1
2̄21	3.5345	17	221̄	3.53	1	402	2.1104	5			
1̄31	3.4992	12	131̄	3.493	1	341	2.0733	7			
211	3.4847	7				431	2.0711	16	341	2.070	2
1̄02	3.3662	15				223	2.0658	27			
131	3.3007	11				052	2.0553	11	061	2.055	1
012	3.2749	65	112̄	3.251	3	421	2.0256	5			
040	3.2333	19				350	2.0022	17			
230	3.1904	6				033	1.9994	8			
300	3.1626	29	300	3.170	2	342	1.9899	24	033, 342̄	1.992	2
221	3.1578	8				161	1.9873	13			
310	3.0721	100	310	3.075	10	260	1.9624	5			
140	3.0604	21				133	1.9020	14	133, 511̄	1.894	1
102	3.0360	12				143	1.8636	22			
2̄31	3.0159	95	102, 231̄	3.019	8	261	1.8519	8	143̄, 261	1.855	1
022	2.9991	27				521	1.8314	29	521̄	1.836	1
202	2.9953	18				520	1.8208	5			
1̄22	2.9858	16				170	1.8135	7			
112	2.9557	40	112	2.936	1	342	1.7867	13	502, 342	1.785	1
041	2.9176	23				360	1.7812	5			
1̄41	2.8453	44	141̄, 320	2.843	5	441	1.7805	12			
320	2.8410	39				171	1.7655	14			
3̄21	2.7678	9	321̄	2.778	1	511	1.7386	9	530, 422	1.739	1
122	2.7482	17	122	2.742	2	004	1.6926	7			
141	2.7355	33				271	1.6925	11			
240	2.6717	5				204	1.6831	6			
032	2.6625	63	032	2.659	3	432	1.6683	7			
050	2.5866	5				243	1.6512	6			
241	2.5667	18	241̄	2.565	1	271	1.6455	6			
202	2.5655	6				362	1.6393	5			
212	2.5164	10				104	1.6214	5			
150	2.4955	5				513	1.5730	9			
132	2.4822	6				163	1.5665	6			
312	2.4779	15	312̄, 132	2.475	1	443	1.5636	6			
2̄32	2.4598	10				620	1.5360	5			
241	2.4110	15				471	1.4551	5			
222	2.3847	7				652	1.3177	6			
1̄51	2.3747	5				660	1.2750	6			
3̄22	2.3518	6	113̄, 420	2.234	1						

1: calculated powder pattern and indexing for dervillite of this study. *d* values calculated on the basis of *a* = 9.6155(7) Å, *b* = 12.9331(8) Å, *c* = 6.8616(5) Å, β = 99.352(8)°, and with the atomic coordinates reported in Table 2. Intensities calculated using *XPOW* software version 2.0 (Downs *et al.*, 1993).

2: observed powder pattern and indexing (converted to the current axes orientation) originally reported by Bari *et al.* (1983).

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