



Title	Cervelleite, Ag <sub>4</sub> TeS: solution and description of the crystal structure
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# Mineralogy and Petrology

## Cervelleite, Ag<sub>4</sub>TeS: solution and description of the crystal structure

--Manuscript Draft--

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<b>Abstract:</b>	Examination of the type specimen of cervelleite throws new light on its structure demonstrating how earlier researchers erred in describing the mineral as cubic. It was found to be monoclinic, space group P21/n, with $a = 4.2696(4)$ , $b = 6.9761(5)$ , $c = 8.0423(7)$ Å, $\beta = 100.332(6)^\circ$ , $V = 235.66(3)$ Å <sup>3</sup> , $Z = 4$ . The crystal structure [ $R1 = 0.0329$ for 956 reflections with $I > 2\sigma(I)$ ] is topologically identical to that of acanthite, Ag <sub>2</sub> S, and aguilrite, Ag <sub>4</sub> SeS. It can be described as a body-centered array of tetrahedrally coordinated X atoms (where X = S and Te) with Ag <sub>2</sub> X <sub>4</sub> polyhedra in planes nearly parallel to (010); the sheets are linked by the other silver position (i.e., Ag1) that exhibits a three-fold coordination. Crystal-chemical features are discussed in relation to other copper and silver sulfides/tellurides, and pure metals. A SEM study of the cervelleite crystal used for the structural investigation showed that it is intergrown with an unnamed Ag <sub>2</sub> FeS <sub>2</sub> phase in the type material.
<b>Response to Reviewers:</b>	Dear Anton, Please find herewith the revised copy of the manuscript entitled "Cervelleite, Ag <sub>4</sub> TeS: solution and description of the crystal structure" by Luca Bindi, Christopher J. Stanley, and Paul G. Spry. We did the minor stylistic changes suggested by the reviewers. We think that it is not necessary to add the Table as suggested by Rev#2.  With best regards, Luca Bindi

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55 **Keywords:** cervelleite · Ag-Te-S system · Ag-Cu sulfotellurides · crystal structure ·  
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## Abstract

Examination of the type specimen of cervelleite throws new light on its structure demonstrating how earlier researchers erred in describing the mineral as cubic. It was found to be monoclinic, space group  $P2_1/n$ , with  $a = 4.2696(4)$ ,  $b = 6.9761(5)$ ,  $c = 8.0423(7)$  Å,  $\beta = 100.332(6)^\circ$ ,  $V = 235.66(3)$  Å<sup>3</sup>,  $Z = 4$ . The crystal structure [ $R1 = 0.0329$  for 956 reflections with  $I > 2\sigma(I)$ ] is topologically identical to that of acanthite,  $\text{Ag}_2\text{S}$ , and aguilarite,  $\text{Ag}_4\text{SeS}$ . It can be described as a body-centered array of tetrahedrally coordinated X atoms (where  $X = \text{S}$  and  $\text{Te}$ ) with  $\text{Ag}_2\text{X}_4$  polyhedra in planes nearly parallel to (010); the sheets are linked by the other silver position (i.e.,  $\text{Ag}1$ ) that exhibits a three-fold coordination. Crystal-chemical features are discussed in relation to other copper and silver sulfides/tellurides, and pure metals. A SEM study of the cervelleite crystal used for the structural investigation showed that it is intergrown with an unnamed  $\text{Ag}_2\text{FeS}_2$  phase in the type material.

## Introduction

Silver chalcogenides have received much attention in recent years because of their important technological applications (e.g., Padma Kumar and Yashonath 2006). These compounds are known to be fast ionic conductors or semiconductors and, as such, find practical applications in silver photography as sensitizers or in optics and microelectronics as rewritable storage media. From a geological standpoint, silver sulfotellurides are trace constituents accompanying native gold and Au-Ag-tellurides in various deposit types that span the magmatic-hydrothermal spectrum.

In the system Ag-Te-S, cervelleite  $\text{Ag}_4\text{TeS}$  is of particular interest because it occurs as an accessory mineral in a range of hydrothermal precious mineral deposits (Cook and Ciobanu 2003). It was defined as a new mineral species by Criddle et al.

1 (1989) during a study of ore minerals collected from the spoil tips of the abandoned  
2 Bambolla mine, Moctezuma, Sonora (Mexico). By means of X-ray photographic  
3 techniques, these authors studied fragments of cervelleite intergrown with acanthite  
4 from a structural point of view and reported a cubic symmetry (with  $P2_3$ ,  $Pm3$ ,  $P4_32$ ,  
5  $P4_3m$ ,  $Pm3m$ ,  $P2_13$ ,  $P4_232$ ,  $P4_132$ ,  $P4_332$ ,  $Pa3$  as possible space groups) with  $a =$   
6  $14.03(1)$  and  $Z = 24$ . Criddle et al. (1989) also noticed that cervelleite, acanthite and  
7 hessite were altered rapidly and profoundly by light, in a surface reaction interpreted  
8 as photo-chemical in origin.  
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19 Cervelleite, along with other cervelleite-like minerals, has been reported from  
20 various ore types including the intrusion-hosted San Martin deposit, Argentina (Paar  
21 and De Brodtkorb 1996), the epithermal Mayflower Au-Ag deposit, Montana (Spry  
22 and Thieben 1996), the Um Samiuki volcanogenic massive sulfide deposit, Egypt  
23 (Helmy 1999), epithermal (Larga, Roşia Montană) and skarn (Băiţa Bihor and Ocna  
24 de Fier) occurrences in Romania (Cook and Ciobanu 2003; Ciobanu et al. 2004), the  
25 Eniovche epithermal deposit, Bulgaria (Dobrev et al. 2002), the intrusion-hosted  
26 Funan Au deposit, China (Gu et al. 2003), and several volcanic-hosted massive  
27 sulfide deposits in the southern Urals (Novoselov et al. 2006). Unnamed Ag-  
28 sulfotellurides  $[(Ag,Cu)_6TeS_2 - (Ag,Cu)_4TeS]$  were described from the Funan deposit  
29 (Gu et al. 2003), and a phase with the composition  $Ag_2Cu_2TeS$  was reported by Cook  
30 and Ciobanu (2003) from the Băiţa Bihor and Ocna de Fier skarns in Romania. In  
31 Greece, cuprian cervelleite and unnamed Ag-Cu sulfotellurides  $[(Ag,Cu)_{12}Te_3S_2$  and  
32  $(Ag,Au,Cu)_9Te_2S_3]$  were described from the intrusion-related deposit at Panormos  
33 Bay, Tinos Island (Tombros et al. 2004, 2010; Spry et al. 2006). In the Kallianou area  
34 (southern Evia Island, Greece), gold-bearing quartz veins contain an exotic ore  
35 mineralogy including cervelleite-like sulfotellurides  $[Ag_2CuTeS$  and  $(Ag,Cu)_2Te]$  and  
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Te-rich polybasite (Voudouris and Spry 2008; Voudouris et al. 2011; Bindi et al. 2013b).

In the course of a research project dealing with the description and structural characterization of natural copper and silver tellurides (Bindi 2008, 2009, 2014; Bindi and Cipriani 2004; Bindi and Pinch 2014; Bindi and Pingitore 2013; Bindi et al. 2004, 2005, 2009, 2013a, 2013b), we have examined a fragment of cervelleite from the holotype material (catalogue number E.1161 BM 1985, 354).

## The holotype

The specimen was collected by the late Alan Criddle on a field excursion to the Sonora Desert led by the late Sid Williams. It consists of black powdery crusts (1–2 mm thick) of benleonardite, acanthite, hessite and cervelleite, together with gangue quartz and dolomite (Fig. 1). The hessite contains a vermiform or myrmekitic intergrowth of fine-grained cervelleite (pale-greenish-grey in Fig. 1). The assemblage occupies irregular fractures in a highly altered rock described by Williams (1982) as an intensely silicified rhyolitic vitrophyre.

## Crystal-structure solution and refinement

A small crystal fragment (40 × 55 × 60 μm) was selected from the type specimen for the X-ray single-crystal diffraction study that was done with an Oxford Diffraction Xcalibur 3 CCD single-crystal diffractometer (Table 1). Surprisingly, most of the X-ray reflections (89% of the total) match the following monoclinic unit cell:  $a \sim 4.30$ ,  $b \sim 6.98$ ,  $c \sim 8.04$  Å and  $\beta \sim 100^\circ$ , being very close to those of acanthite, Ag<sub>2</sub>S (Frueh 1958) and aguilarite (Bindi and Pingitore 2013). The other 11% of the total reflections could be indexed according to the following monoclinic (primitive) unit cell:

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$a \sim 9.00$ ,  $b \sim 12.56$ ,  $c \sim 5.76$  Å,  $\beta = 94^\circ$  (*vide infra*). The data were reduced taking into account the first monoclinic cell. Systematic absences ( $h0l$ :  $h + l = 2n$ ;  $h00$ :  $h = 2n$ ;  $0k0$ :  $k = 2n$ ;  $00l$ :  $l = 2n$ ) were consistent with the space groups  $P2_1/n$  ( $P2_1/c$  as standard). Statistical tests on the distribution of  $|E|$  values strongly indicate the presence of an inversion centre ( $|E^2-1| = 0.922$ ), thus supporting the choice of the space group  $P2_1/n$ . We decided to refine the cervelleite structure in the non-standard space group  $P2_1/n$  in order to have the same orientation reported for acanthite and aguilarite. The program SHELXL (Sheldrick 2008) was used for the refinement of the structure, which was carried out starting from the atomic coordinates of acanthite by Frueh (1958). The occupancy of all the sites was left free to vary (Ag vs. vacancy; Te vs. S) and then fixed to the resulting value. The refined values are given in Table 2. Neutral scattering curves for Ag, S and Te 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 atoms and no constraints, the residual value settled at  $R = 0.0298$  for 418 observed reflections [ $2\sigma(I)$  level] and 29 parameters and at  $R = 0.0329$  for all 956 independent reflections. Experimental details and  $R$  indices are given in Table 1. Fractional atomic coordinates and isotropic displacement parameters are reported in Table 2 (anisotropic ADPs can be found in the accompanying CIF). Bond distances are given in Table 3. The calculated X-ray powder-diffraction pattern, computed with the atom coordinates and occupancies reported in Table 2, is given in Table 4. Structure factors and CIF are available from the authors upon request.

## Results and Discussion

### Description of the crystal structure

1 The crystal structure of cervelleite (Fig. 2) is topologically identical to that of  
 2 acanthite (Frueh 1958) and aguilarite (Bindi and Pingitore 2013). It can be described  
 3 as a body-centered array of tetrahedrally coordinated X atoms (where X = S, Se and  
 4 Te) with Ag<sub>2</sub>-polyhedra in planes nearly parallel to (010); the sheets are linked by the  
 5 other silver position (i.e., Ag1) that exhibits a three-fold coordination. Due to the  
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Te) with Ag<sub>2</sub>-polyhedra in planes nearly parallel to (010); the sheets are linked by the other silver position (i.e., Ag1) that exhibits a three-fold coordination. Due to the greater size of Te compared to S and Se, Ag1 and Ag2 atoms in cervelleite increase their coordination number to 3 and 4, respectively, with respect to that observed in acanthite and aguilarite (2 and 3 for Ag1 and Ag2, respectively). Results indicate that  $Z = 4$  [with an unit-cell volume of  $235.66(3) \text{ \AA}^3$  and formula  $\text{Ag}_2(\text{Te}_{0.50}\text{S}_{0.50})$ ], unlike the findings of Criddle et al. (1989) that reported  $Z = 24$  [with unit-cell volume of  $2762(2) \text{ \AA}^3$  and formula  $\text{Ag}_4\text{TeS}$ ]. As such, the computed density should be  $8.247 \text{ g/cm}^3$  rather than the value of  $8.53 \text{ g/cm}^3$  reported previously.

In the structure, the bond distances observed for the two silver positions (i.e.,  $\langle \text{Ag1-X} \rangle = 2.660 \text{ \AA}$  and  $\langle \text{Ag2-X} \rangle = 2.729 \text{ \AA}$ ) are larger than those observed in acanthite [ $\langle \text{Ag1-X} \rangle = 2.503 \text{ \AA}$  and  $\langle \text{Ag2-X} \rangle = 2.602 \text{ \AA}$ , Frueh (1958)] and aguilarite [ $\langle \text{Ag1-X} \rangle = 2.511 \text{ \AA}$  and  $\langle \text{Ag2-X} \rangle = 2.628 \text{ \AA}$ , Bindi and Pingitore (2013)], due to the greater size of Te compared to Se and S (Shannon 1976). On the whole, the observed Ag–X bond distances (Table 3) are intermediate with respect to the Ag–Te distances observed in hessite,  $\text{Ag}_2\text{Te}$  (2.84–3.03  $\text{ \AA}$ ; Van der Lee and de Boer 1993), sylvanite,  $(\text{Au,Ag})_2\text{Te}_4$  (2.74–3.23  $\text{ \AA}$ ; Pertlik 1984), muthmannite,  $\text{AuAgTe}_2$  (2.69–2.97  $\text{ \AA}$ ; Bindi and Cipriani 2004), and empressite,  $\text{AgTe}$  (2.84–2.96  $\text{ \AA}$ ; Bindi et al. 2004), and those observed for some Ag–Se minerals (e.g., naumannite,  $\text{Ag}_2\text{Se}$ , 2.62–2.86  $\text{ \AA}$ , Wieggers 1971; aguilarite,  $\text{Ag}_4\text{SeS}$ , 2.51–2.63  $\text{ \AA}$ , Bindi and Pingitore 2013).



1 The shortest Ag–Ag contact in cervelleite ( $\text{Ag}_2\text{–Ag}_2 = 2.968 \text{ \AA}$ ) is nearly  
2 identical to the corresponding value in naumannite ( $\text{Ag–Ag} = 2.93 \text{ \AA}$ , Wiegiers 1971),  
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4 and is very similar to those observed in *fcc* silver ( $\text{Ag–Ag} = 2.89 \text{ \AA}$ ; Suh et al. 1988)  
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6 or *hcp* silver [ $\text{Ag–Ag} = 2.93 \text{ \AA}$ ; Petruk et al. 1970]. The mean electron number refined  
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8 for the X position [ $0.527(3)\text{Te} + 0.473\text{S} = 34.97$ ] is in excellent agreement with the  
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10 chemical formula reported in the literature for cervelleite, i.e.  $\text{Ag}_4\text{TeS}$ .  
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14 In Figure 3, the unit-cell volumes of synthetic members belonging to the two  
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16 solid solutions, the monoclinic ‘acanthite-like’  $\text{Ag}_2\text{S} - \text{Ag}_2\text{S}_{0.4}\text{Se}_{0.6}$  series and the  
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18 orthorhombic ‘naumannite-like’  $\text{Ag}_2\text{S}_{0.3}\text{Se}_{0.7} - \text{Ag}_2\text{Se}$  series (Pingitore et al. 1992),  
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20 are plotted against the selenium contents. A good linear trend is observed  
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22 corresponding to the expansion of the lattice dimensions as the larger  $\text{Se}^{2-}$  anion  
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24 replaces  $\text{S}^{2-}$ , following Vegard’s law for the properties of solid solutions. Taking into  
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26 consideration the ionic radii of Te, Se and S, if we calculate a mean value for  
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28 cervelleite ( $\text{Te}_{0.50}\text{S}_{0.50}$ ) and then extrapolate the potential amount of Se (to plot it in  
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30 Figure 3), we can see that the studied crystal (filled circle) occurs along this trend.  
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40 Discussion of the previous results obtained by Criddle et al. (1989)  
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42 We have here unambiguously shown for the first time that cervelleite represents  
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44 the Te-analogue of aguilarite. However, a puzzling aspect of the current study is that  
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46 Criddle et al. (1989) described cervelleite as an optically isotropic mineral with a  
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48 cubic symmetry. We note here that the same set of *d* spacings reported by Criddle et  
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50 al. (1989), which are indexed with a primitive cubic lattice with  $a = 14.03 \text{ \AA}$ , can be  
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52 obtained with the monoclinic unit cell found in this study and matching the 11% of the  
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54 total reflections collected from our ‘cervelleite’ crystal. The refined monoclinic unit cell  
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56 can be written as  $a = 8.994(8)$ ,  $b = 12.56(1)$ ,  $c = 5.761(6) \text{ \AA}$ ,  $\beta = 93.90(8)^\circ$ ,  $V =$   
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649.3(9) Å<sup>3</sup> and the comparison with the diffraction pattern originally reported by Criddle et al. (1989) is given in Table 5.

We surmise that Criddle et al. (1989) obtained chemical and optical data on cervelleite but carried out X-ray data on this second monoclinic unknown phase. This unknown phase is intergrown with cervelleite, and occurs in variable amounts. To corroborate these findings, we embedded the cervelleite grain in epoxy used for the structural investigation and studied the polished section by means of a scanning electron microscope. The grain appears to be formed of two phases (Fig. 4): a brighter phase which shows the composition typically observed for cervelleite (i.e., Ag<sub>4</sub>TeS, when the data are normalized on the basis of 6 atoms per formula unit), and a darker phase with stoichiometry Ag<sub>2</sub>FeS<sub>2</sub>, which is likely responsible for the diffraction peaks belonging to the second monoclinic unit cell [i.e.,  $a = 8.994(8)$ ,  $b = 12.56(1)$ ,  $c = 5.761(6)$  Å,  $\beta = 93.90(8)^\circ$ ]. Unfortunately, the very low number of reflections for this unnamed Ag<sub>2</sub>FeS<sub>2</sub> phase precludes any *ab initio* structure determination. The search for grains composed of this potential new mineral only failed.

Thus, the holotype sample contains cervelleite, benleonardite and an unknown (likely) new Ag-Fe-S phase exhibiting the second monoclinic unit-cell identified here (which replaced the cubic cell given by Criddle et al. 1989).

## Conclusions

1. Cervelleite is monoclinic, space group  $P2_1/n$ , with  $a = 4.2696(4)$ ,  $b = 6.9761(5)$ ,  $c = 8.0423(7)$  Å,  $\beta = 100.332(6)^\circ$ ,  $V = 235.66(3)$  Å<sup>3</sup>,  $Z = 4$ . The crystal structure [ $R1 = 0.0329$  for 956 reflections with  $I > 2\sigma(I)$ ], solved for the first time, demonstrates that the mineral is the Te-analogue of aguilrite.

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2. Cervelleite coexists with an unnamed  $\text{Ag}_2\text{FeS}_2$  phase in the type sample. The unnamed phase exhibits a monoclinic symmetry with cell dimensions:  $a = 8.994(8)$ ,  $b = 12.56(1)$ ,  $c = 5.761(6)$  Å,  $\beta = 93.90(8)^\circ$  and  $V = 649.3(9)$  Å<sup>3</sup>. The comparison with the diffraction pattern originally reported by Criddle et al. (1989) gave an excellent match.
  3. The museum specimen studied here (catalogue number E.1161 BM 1985, 354) is the type sample for cervelleite, benleonardite and a new previously unidentified Ag-Fe-S phase.

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## Figure Captions

1  
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3  
4 Figure 1 – Reflected plane polarized light digital image (in oil immersion) illustrating  
5  
6 pale greenish cervelleite overgrowths on acanthite rosettes (with intergrown  
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8 unknown phase) and coarser acanthite (near scale bar) and quartz (middle  
9  
10 left). Creamy white hessite forms the infill. The sample (catalogue number  
11  
12 E.1161 BM 1985, 354) is the type specimen for both cervelleite and  
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14 benleonardite.  
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19 Figure 2 – The crystal structure of cervelleite projected down [100]. The horizontal  
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21 direction is the *c* axis. Ag and X (S and Te) are given as white and black  
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23 spheres, respectively. The unit cell is outlined.  
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27 Figure 3 – The unit-cell volume ( $\text{\AA}^3$ ) plotted against the Se content (a.p.f.u.). Filled  
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29 symbol represents the cervelleite crystal (this study), whereas empty symbols  
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31 are data from synthetic compounds (Pingitore et al. 1992).  
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35 Figure 4 – SEM-BSE image showing the coexistence of two phases (brighter:  
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37 cervelleite, darker: unnamed  $\text{Ag}_2\text{FeS}_2$ ) in the crystal used for the structural  
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39 investigation.  
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**TABLE 1** – Crystallographic data and refinement parameters for cervelleite

<b>Crystal data</b>			
Ideal formula	Ag <sub>4</sub> TeS		
Crystal system	monoclinic		
Space group	<i>P2<sub>1</sub>/n</i>		
Unit-cell parameters (Å, °)	4.2696(4)	6.9761(5)	8.0423(7)
Unit-cell volume (Å <sup>3</sup> )	90.00	100.332(6)	90.00
Z	4		
Crystal size (mm)	0.060×0.055×0.040		
<b>Data collection</b>			
Diffractometer	Oxford Xcalibur 3		
Temperature (K)	293(2)		
Radiation, wavelength (Å)	MoKα 0.71073		
2θ max for data collection (°)	69.96		
Crystal-detector dist. (mm)	50		
<i>h, k, l</i> ranges	-6 – 6, -11 – 11, -12 – 12		
Axis, frames, width (°), time per frame (s)	ω/φ, 1211, 1.00, 70		
Total reflections collected	3911		
Unique reflections ( <i>R</i> <sub>int</sub> )	956 (0.041)		
Unique reflections <i>I</i> > 2σ( <i>I</i> )	418		
Data completeness to θ <sub>max</sub> (%)	99.6		
Absorption correction method	ABSPACK (Oxford Diffraction 2006)		
<b>Structure refinement</b>			
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>		
Data/restraints/parameters	956/0/29		
<i>R</i> <sub>1</sub> [ <i>I</i> > 2σ( <i>I</i> )], <i>wR</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0298, 0.0560		
<i>R</i> <sub>1</sub> all, <i>wR</i> <sub>2</sub> all	0.0329, 0.0562		
Goodness-of-fit on <i>F</i> <sup>2</sup>	0.975		
Largest diff. peak and hole (e <sup>-</sup> /Å <sup>3</sup> )	0.76, -0.45		

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

$$R_1 = \sum || F_o | - |F_c|| / \sum | F_o | \quad wR_2 = \left\{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \right\}^{1/2}$$

$$GooF = \left\{ \sum [w(F_o^2 - F_c^2)^2] / (n-p) \right\}^{1/2} \quad \text{where } n = \text{no. of reflections, } p = \text{no. of refined parameters}$$

**TABLE 2** – Atoms, Wyckoff letter, site occupancy, fractional atom coordinates (Å), and isotropic atomic displacement parameters (Å<sup>2</sup>) for cervelleite

atom	Wyckoff	site occupancy	x	y	z	$U_{\text{eq}}$
Ag1	4e	Ag <sub>1.00</sub>	0.7542(3)	0.0339(1)	0.34094(8)	0.0244(2)
Ag2	4e	Ag <sub>1.00</sub>	0.2887(2)	0.3487(1)	0.41168(8)	0.0261(2)
X	4e	Te <sub>0.527(3)</sub> S <sub>0.473</sub>	0.3608(2)	0.2417(2)	0.13068(9)	0.0296(3)

**TABLE 3** – Selected bond distances (Å) for cervelleite

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Ag1 - X	2.600(1)	Ag2 - X	2.451(1)	Ag1 -Ag2	3.041(1)
- X	2.603(1)	- X	2.815(1)	-Ag2	3.079(1)
- X	2.776(1)	- X	2.821(1)	-Ag2	3.083(1)
<Ag1-X>	2.660	- X	2.827(1)	-Ag2	3.145(1)
		<Ag2-X>	2.729	-Ag2	3.321(1)
				Ag2 -Ag2	2.968(1)

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**TABLE 4** – Calculated powder diffraction pattern for cervelleite

<i>h</i>	<i>k</i>	<i>l</i>	<i>I</i> <sub>calc</sub>	<i>d</i> (Å)
1	1	1	21	3.1009
-1	1	2	100	2.8923
1	2	0	61	2.6834
-1	2	1	43	2.6347
0	2	2	8	2.6163
1	1	2	56	2.4791
0	1	3	23	2.4669
1	2	1	71	2.4571
-1	0	3	33	2.4392
0	3	1	39	2.2310
0	2	3	13	2.1037
2	0	0	37	2.1002
1	0	3	6	2.0724
-1	3	1	6	2.0129
2	1	0	19	2.0110
0	3	2	36	2.0047
-1	2	3	19	1.9989
1	1	3	17	1.9866
0	0	4	29	1.9780
-2	1	2	10	1.9317
0	3	3	9	1.7442
-2	2	2	12	1.7417
0	4	1	7	1.7031
-1	2	4	8	1.6872
-1	4	1	8	1.6000
-2	0	4	11	1.5892
-2	3	1	7	1.5693
-2	3	2	6	1.5208
2	3	1	11	1.4920
-1	3	4	9	1.4841
2	1	3	7	1.4812
-1	2	5	5	1.4370
-2	3	3	8	1.4276
-3	1	2	8	1.3739
1	3	4	8	1.3603
-2	4	1	6	1.3486
-1	5	1	12	1.3181
3	1	1	7	1.3142
2	1	4	7	1.3028
1	2	5	7	1.2995
1	5	1	7	1.2941
2	4	2	7	1.2285
-2	2	6	7	1.1513
-3	4	1	7	1.1026

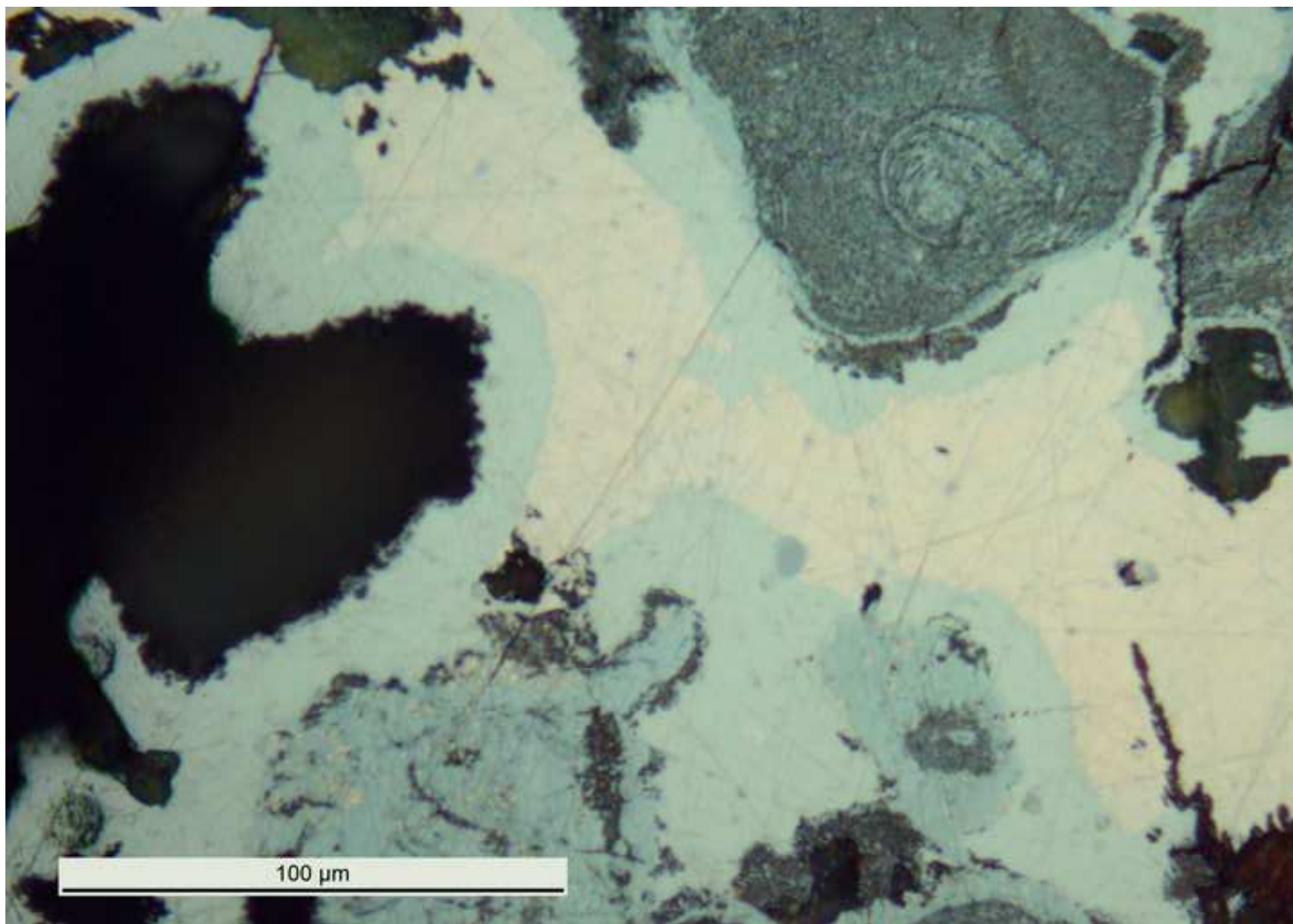
*d* values calculated on the basis of  $a = 4.2694(4)$ ,  $b = 6.9761(5)$ ,  $c = 8.0423(7)$  Å,  $\beta = 100.332(6)^\circ$ , and with the atomic coordinates and occupancies reported in Table 2.

Intensities calculated using XPOW software version 2.0 (Downs et al. 1993). Only  $I > 5\sigma(I)$  are reported.

**TABLE 5** – X-ray powder diffraction patterns for the unnamed  $\text{Ag}_2\text{FeS}_2$  phase intergrown with cervelleite

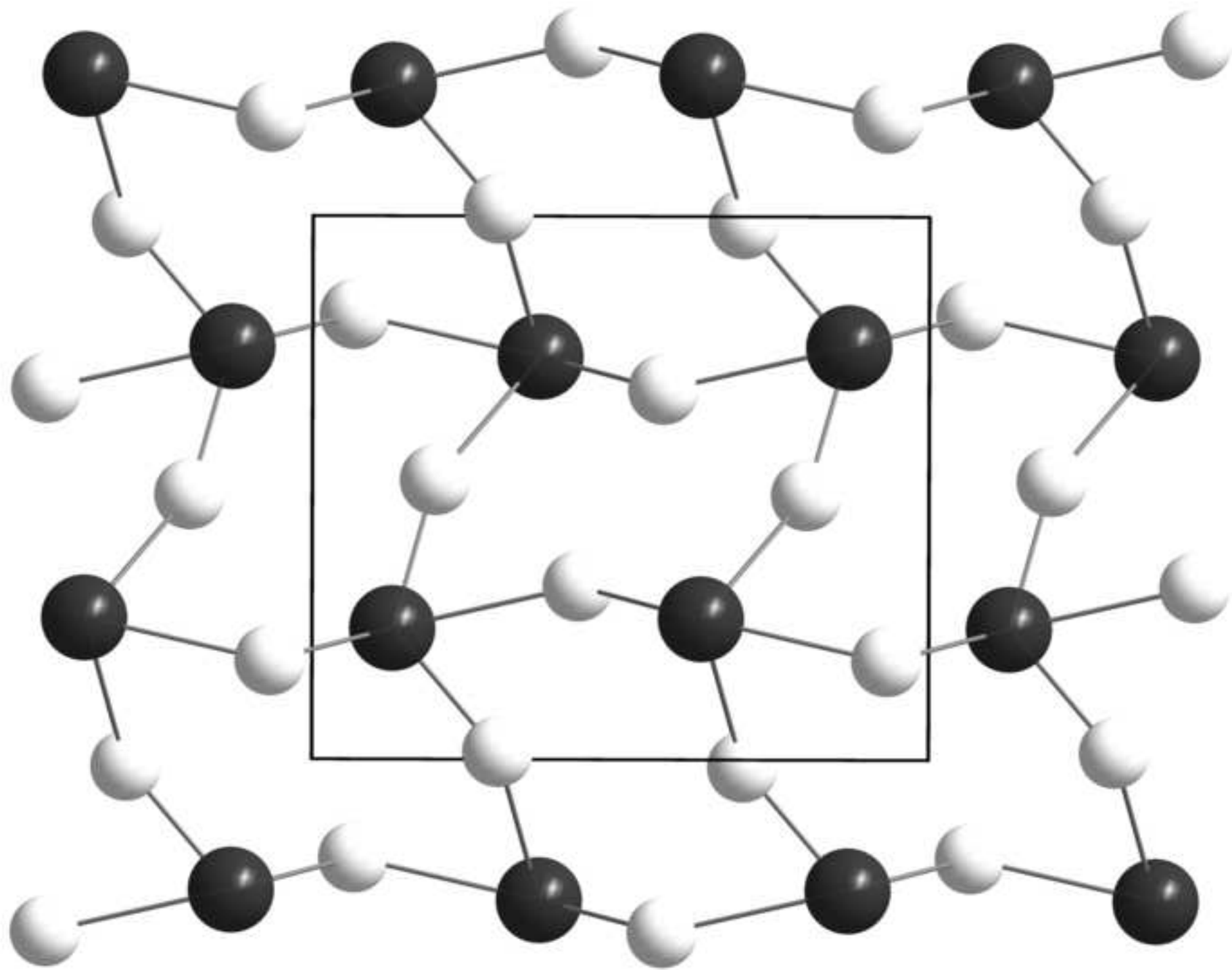
<i>hkl</i>	1		2		
	$d_{obs}$ (Å)	$I_{obs}$	$I_{obs}$	$d_{obs}$ (Å)	$I_{obs}$
020	6.28	60	012	6.29	s
001	5.75	10	112	5.74	w
-101	5.00	100	022	5.00	vvs
-111	4.643	35	122,003	4.64	m
021	4.240	80	113	4.24	vs
121	3.761	35	123	3.766	ms
201	3.425	5	014,223	3.421	vw
230	3.061	5	–	–	–
-231	2.755	2	134,015	2.753	vw
311	2.529	5	n.i.	2.530	vw
212	2.308	10	016	2.304	w
-401	2.140	5	335	2.137	vw
-251	2.071	5	–	–	–
251	2.026	5	444	2.026	vw
061	1.9670	10	117,155	1.9659	vw
350	1.9242	5	146,027	1.9247	vw
-261	1.8170	5	n.i.	1.8174	vw

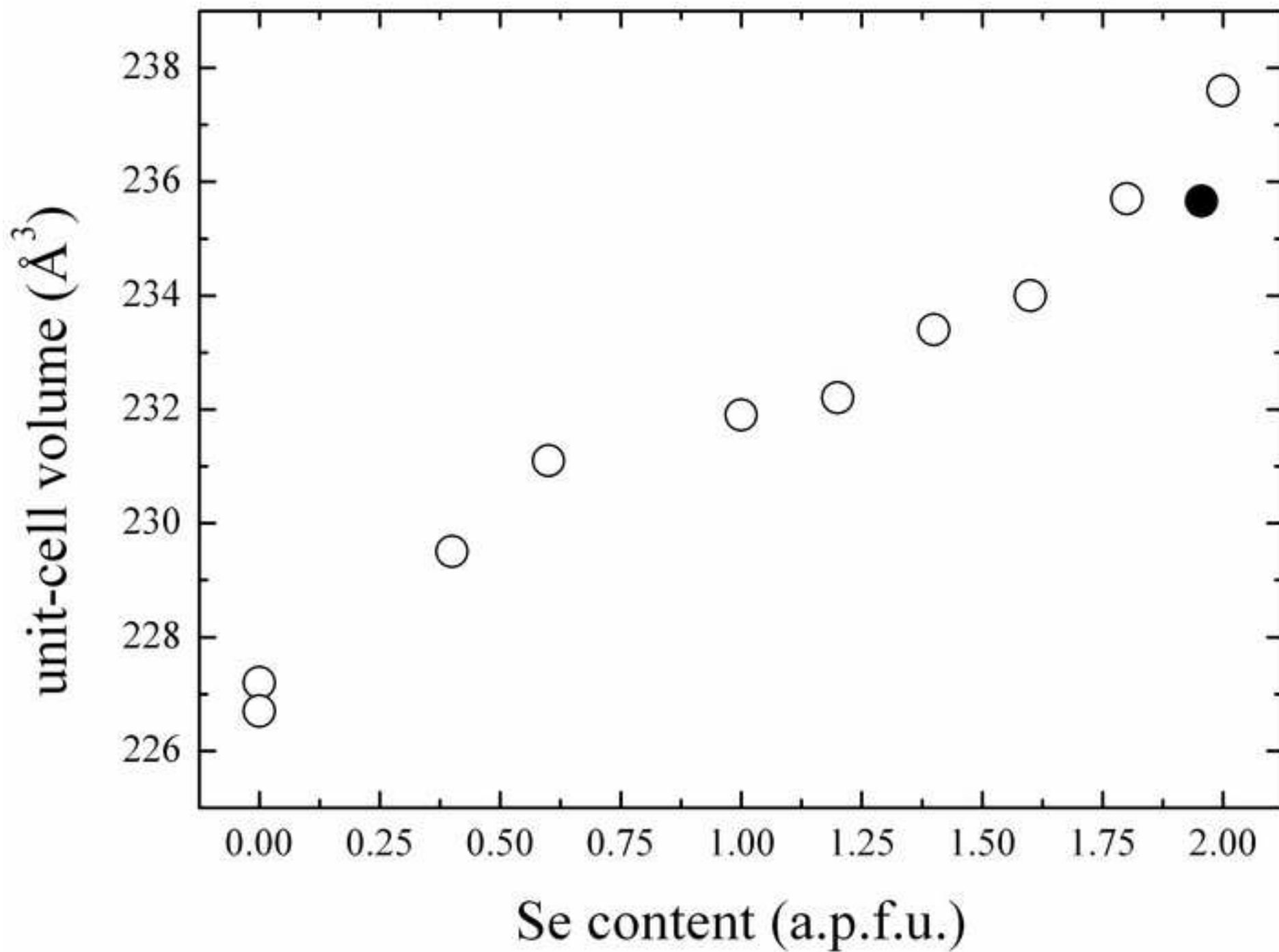
*Note:* 1 = observed powder pattern of the unnamed  $\text{Ag}_2\text{FeS}_2$  phase of this study. 2 = observed powder pattern and indexing originally reported by Criddle et al. (1989) for ‘cervelleite’.





Line Figure  
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