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THE ROLE OF THE Sb^{3+} LONE-ELECTRON PAIRS AND Fe^{2+} COORDINATION IN THE HIGH-PRESSURE BEHAVIOR OF BERTHIERITE

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ABSTRACT

A single crystal of natural berthierite, $FeSb_2S_4$, was investigated at high pressure by means of X-ray diffraction using a diamond-anvil cell equipped with diamond backing plates. No phase transitions were indicated up to 8 GPa. The third-order Birch–Murnaghan equation of state, calculated using high-accuracy volume–pressure data up to 8.05 GPa, gave the following coefficients: V_0 = 608.78(7) Å^3, K_{T0} = 37.2(2) GPa and K' = 7.0(1). The evolution of the structure as a function of pressure has been determined at seven different pressures up to 7.41 GPa. As in other structures with stereochemically active lone-electron pairs (LEP), the Sb^{3+} LEP, influencing long Sb–S bonds in berthierite, accommodate most of the compression. The Fe octahedron, which is the stiffest coordination polyhedron in berthierite, increases its distortion until approximately 5 GPa, but shows pronounced stiffening at higher pressures. This deformation at high pressures can be related to an increase in the Jahn–Teller effect on the Fe^{2+} coordination. The influence of Fe on compressional behavior makes a distinct difference between the compression of berthierite and that of stibnite, Sb_2S_3. The bridging Fe coordination between the structural rods in berthierite makes it stiffer. This, together with the direct structural relation to the analogous $PbBi_2S_4$, galenobismutite, makes the compressional characteristics of berthierite more akin to those of galenobismutite, despite quantitative differences in the stereochemical expression of the LEP of Sb^{3+} and Bi^{3+}.

Keywords: berthierite, equation of state, crystal structure, high pressure, lone-electron pair, sulfosalts.

INTRODUCTION

The structure of berthierite, a sulfosalt of composition $FeSb_2S_4$, has been determined in space group *Pnam* and refined at ambient temperature by Buerger & Hahn (1955) and later by Bente & Edenharter (1989), Lemoine *et al.* (1991) and Lukaszewicz *et al.* (2001). It presents several interesting aspects. It is a complex sulfide of iron studied for its magnetic properties (Winterberger & André 1990) and considered to undergo a phase transition in the temperature range 323–365 K according to Mössbauer spectra, but without significantly changing the crystal-structure parameters (Lukaszewicz *et al.* 2001). Moreover, the berthierite structure has antimony in a trivalent state and is influenced by its lone-electron pair (LEP), with a pronounced steric effect.

The crystal structure of berthierite belongs to the group of rod-based sulfosalt structures (Makovicky 1993; Fig. 1). It shows several interesting relations to sulfosalts of other structural families. The structural rods in berthierite, which run parallel to the short axis **c**, are interconnected to layers. The 2 Å (1/2 period) relative displacement (shear) of these layers relate berthierite to the meneghinite structural family (Makovicky 1985), to which belongs stibnite, among other structures. On the other hand, berthierite has the same space-group symmetry and its atoms occupy the same Wyckoff positions as in the crystal structure of galenobismutite. Both structures are in isopointal relation to the $CaFe_2O_4$ structure type. Owing to differences in interatomic distances and consequent distribution of chemical bonds, however, berthierite and galeno-

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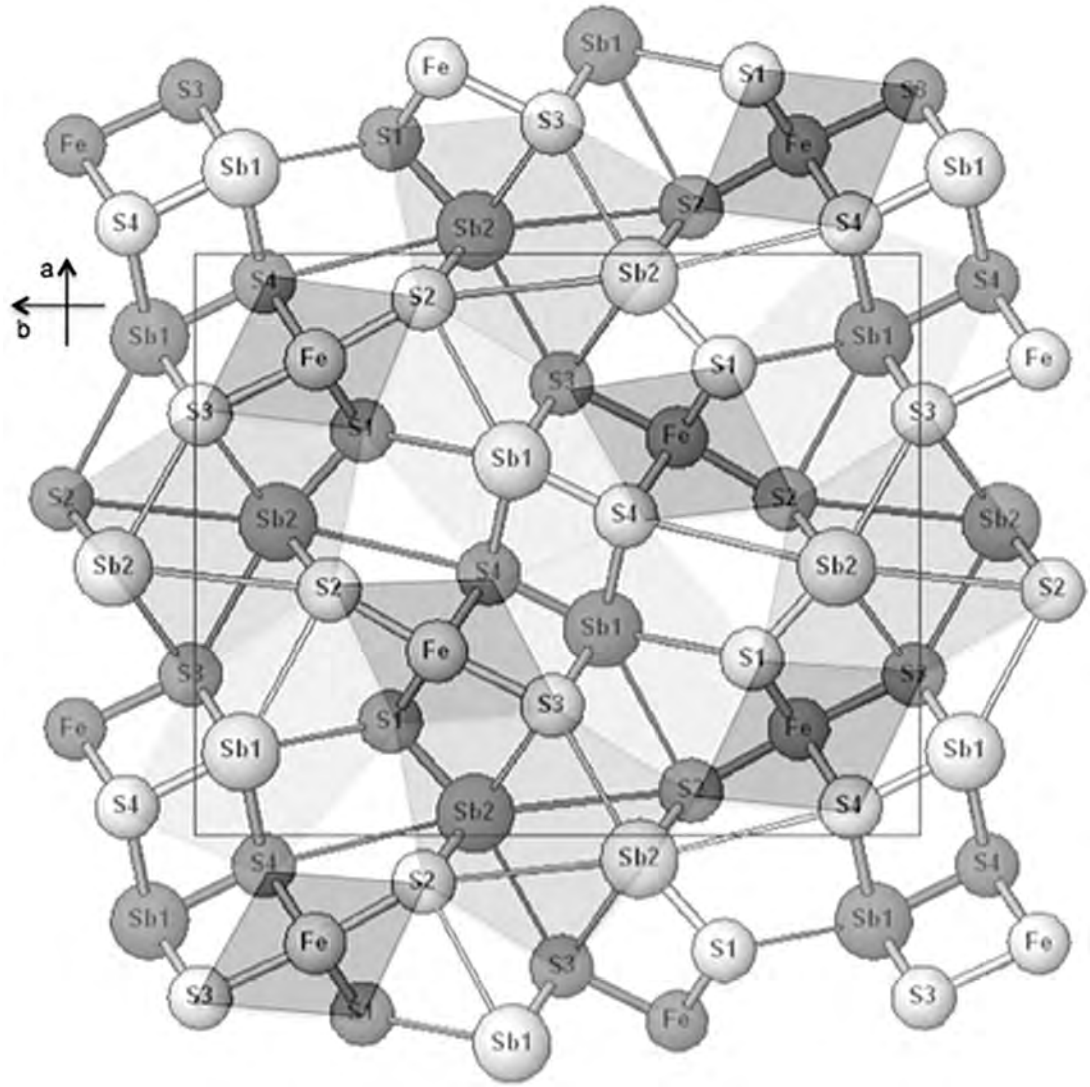


FIG. 1. Crystal structure of berthierite at ambient pressure. Grey circles represent atoms on the $z = 0.25$ mirror plane, and white circles represent atoms on the $z = 0.75$ mirror plane. The bicapped trigonal prisms (Sb1) are shaded light grey, the monocapped trigonal prisms (Sb2) are stippled, and the octahedra (Fe) are dark grey.

bismutite are classified in different sulfosalt structural families (Makovicky 1997).

Among the sulfosalts and sulfides of elements with lone-electron pairs (LEP), studies of the structural behavior under compression by single-crystal X-ray diffraction have been performed so far for stibnite (Sb_2S_3; Lundegaard *et al*. 2003), bismuthinite (Bi_2S_3; Lundegaard *et al*. 2005), galenobismutite ($PbBi_2S_4$; Olsen *et al*. 2007), lillianite ($Pb_3Bi_2S_6$; Olsen *et al*. 2008), heyrovskyite ($Pb_6Bi_2S_9$; Olsen *et al*. 2011) and the high-pressure form of galena (PbS; Grzechnik & Friese 2010). For those minerals, quantitative and detailed measurements of the stereochemical activity of LEP were provided on the basis of calculations of various geometrical parameters of the crystal structure. For bismuthinite also, a theoretical *ab initio* quantum physical study on the effects of compression was made (Olsen *et al*. 2010). In the present study, high-pressure single-crystal X-ray-diffraction experiments have been performed on a natural sample of berthierite in order to determine its equation of state and the high-pressure evolution of the crystal structure at room temperature.

We also discuss the structural relations of berthierite to stibnite and galenobismutite, and we compare the high-pressure behavior of these three structurally related minerals.

Experimental Methods

Two needle-like single crystals of berthierite were selected from a natural sample collected in the hydrothermal vein-type deposit of Herja in the Baia Mare metallogenic area, Romania (Cook & Damian 1997). The first one (183 × 80 × 40 μm) was used for high-pressure determination of the unit-cell dimensions, and we used the other one (175 × 75 × 40 μm) for the collection of intensity data. We used a different crystal for the structural analysis because the first one showed broadened peaks once the pressure was released to atmospheric pressure. The crystals were selected on the basis of their size, lack of twinning, and sharp diffraction profiles. High-pressure single-crystal diffraction experiments were performed in an ETH-type diamond-anvil cell (DAC) equipped with diamond backing plates (Miletich *et al*. 2000, Periotto *et al*. 2011). Stainless steel gaskets pre-indented to a thickness of 90 mm and with a spark-eroded hole 250 mm in diameter were used. A mixture of methanol and ethanol (4:1) was used as the pressure-transmitting medium.

For the pressure–volume equation of state (EoS), the sample was loaded together with a single crystal of quartz used as an internal pressure standard (Angel *et al*. 1997). The measurements of the lattice parameters of the crystal were carried out on a four-circle STOE STADI–IV diffractometer equipped with a point detector and controlled by the SINGLE software (Angel & Finger 2011). The data were acquired using Mo*K*α radiation at 50 kV and 40 mA. Unit-cell parameters were determined from the centering of at least 22 reflections for each high-pressure experiment, in the 2θ range between 11° and 25°. Typical half-widths of reflections were between 0.09° and 0.10° in ω. Full details of the instrument and the peak-centering algorithms are provided in Angel *et al*. (2000). During the centering procedure, the effects of crystal offsets and diffractometer aberrations were eliminated from the refined positions of the peaks using the eight-position centering method (King & Finger 1979). Unconstrained unit-cell parameters, obtained by vector least-squares (Ralph & Finger 1982), were measured at 13 different pressures from room pressure up to 8.046(12) GPa.

The crystal selected for structure analysis was measured from room pressure up to 7.41 GPa, including a measurement on decompression, and loaded in the same DAC as used for the EoS determination. We decided not to load any internal pressure standard in the DAC and used the EoS previously determined in this work for the pressure calibration, as done in a previous investigation (Nestola *et al*. 2008). Complete collections of intensity data were performed using a STOE STADI–IV four-circle diffractometer equipped with Mo*K*α radiation and a CCD detector. The measurements were made in 14 separate ω scans with 1° steps up to 60° in 2θ, using an exposure time of 70 s. The sample–detector distance was 60 mm, and the diffractometer was operated at 50 kV and 40 mA. Data were integrated with the CrysAlis RED software (Oxford Diffraction) and corrected for absorption using the ABSORB software (Angel 2004). Weighted structural refinements were done using the SHELX–97 package (Sheldrick 2008) and were performed in the space group *Pnam*, starting from the atom coordinates of Lemoine *et al*. (1991). The refinements of the anisotropic displacement parameters of atoms showed some problems related to the crystal orientation in the DAC, lying on its (010) face. The lack of information in the direction of the **b** axis is evident because the available *hkl* range is relatively limited for the *k* index, taking in consideration the size of the period in this direction. Therefore, only cation sites were refined with anisotropic displacement parameters, and for the data acquired at a pressure of 2.63 and 6.62 GPa, an isotropic refinement was necessary also for cations because their anisotropic atomic displacement parameters refined as non-positive definite.

Results

Equation of state

The unit-cell parameters and volumes measured at different pressures are reported in Table 1. A continuous decrease of the unit-cell parameters and volumes is observed as a function of pressure, with no evidence of phase transitions up to the maximum pressure reached (Fig. 2). This is also confirmed by the crystal-structure data. From Figure 2a, it is evident that the short **c** axis perpendicular to the mirror plane is the least compressible direction owing to the strongly bonded rods oriented parallel to [001]. On the other hand, the **b** direction undergoes the maximum compression in berthierite, as the LEP are pointing approximately along the [010] direction. The pressure–volume data reported in Table 1 were fitted using a third-order Birch–Murnaghan equation of state (BM3–EoS, Fig. 2b; Birch 1947), refining simultaneously the unit-cell volume (V_0), the bulk modulus (K_{T0}) and its first derivative (K'). By using the EoSFIT5.2 software (Angel 2002), we obtained the following coefficients: V_0 = 608.78(7) Å^3, K_{T0} = 37.2(2) GPa and K' = 7.0(1). These parameters are reported in Table 2, together with the refined BM3–EoS coefficients refined for the unit-cell parameters *a*, *b* and *c*. The F_E–f_E plot (Fig. 3; Angel 2000), based on the finite strain f_E ($[(V_0/V)^{2/3} - 1]/2$) and the normalized stress F_E $[P/3f_E(1 + 2f_E)^{5/2}]$, indicates that the BM3–EoS used for the refinements is appropriate. For the data of this work, the F_E–f_E plot shows that all the data lie on

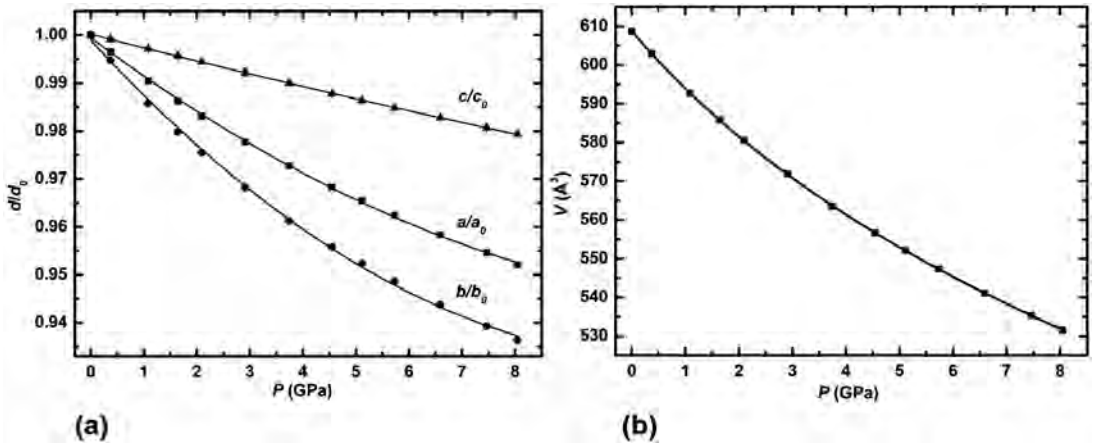


FIG. 2. (a) Evolution of the unit-cell parameters reported as relative compression (d/d_0) as a function of pressure. (b) Evolution of the unit-cell volume as a function of pressure. The solid line represents the fit of a third-order Birch–Murnaghan EoS to the measured data using the EoS coefficients reported in Table 2. The standard deviations are smaller than the symbols used.

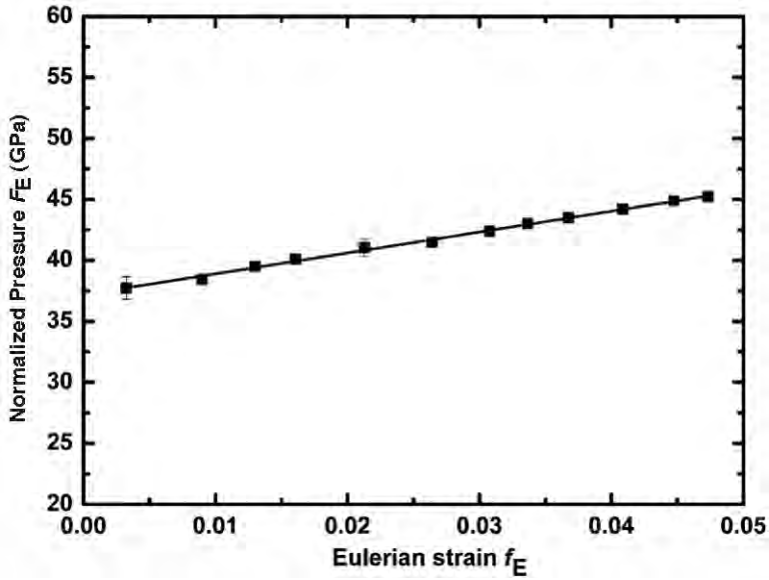


FIG. 3. Normalized pressure F_E *versus* Eulerian strain f_E calculated for the *P*–*V* data. The solid line is a weighted linear regression through the data points and yields the intercept value K_{T0} = 37.2(2) GPa. Its slope gives rise to a *K*' value of 7.07(9).

an inclined straight line. From the *y*-axis intercept and slope [equal to $3K_{T0}(K' - 4)/2$] of such linear fit, we obtain K_{T0} = 37.2(2) and *K*' = 7.07(9), indicating that BM3 is a good choice to fit our *P*–*V* data. The data in Table 2 confirm that the **b** axis is the softest one, with a bulk modulus of 22.1 GPa *versus* 34.9 GPa and 117 GPa for **a** and **c**, respectively. This also results from the different values of *K*', which is much greater for the **b** axis (6.32 compared to 2.5 for the **c** axis).

Table 3 shows the EoS parameters obtained for berthierite and previous results on some related sulfides. An empirical equation from Olsen *et al*. (2007) combines the bulk modulus of sulfides with that of the corresponding sulfosalts. For galenobismutite (Olsen

et al. 2007), using the equation $K_{PbBi2S4} = (2K_{Bi2S3} + K_{PbS})/3$, a value of 41.7 GPa is obtained, which is very close to the observed one. In order to test the same relationship for berthierite, a similar equation can be written: $K_{FeSb2S4} = (2K_{Sb2S3} + K_{FeS})/3$. In this case, the resulting value is 45.3 GPa, significantly different from the one experimentally determined (37.2 GPa). We note that the K_{T0} value of troilite was determined with a much higher standard deviation than the values for sulfosalts and sulfides of metalloids in Table 3. Nevertheless, it seems obvious that the real K_{T0} of berthierite is significantly lower than predicted from the simple empirical relation. It is evident that the LEP compression dominates the behavior much more than the coordination of iron. On the other hand, berthierite is significantly stiffer than stibnite, which has isolated tightly bonded rods in its structure. As seen from Figure 4, contrary to stibnite where the tightly bonded rods are isolated, the rods in berthierite are connected through the Fe coordination polyhedra, and here the loosely bonded spaces influenced by the LEP of Sb^{3+} atoms appear as isolated rods. As a consequence, whereas the rotation of rods and compression of inter-rod spaces in stibnite depend solely on the compression of LEP, in berthierite this effect is largely limited by the Fe coordination polyhedra. We elaborate the differences in the compressional behavior of these two structures further in the following paragraphs.

TABLE 1. UNIT-CELL PARAMETERS OF $FeSb_2S_4$ AT DIFFERENT PRESSURES

P (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
0.0000(1)	11.4164(3)	14.1705(9)	3.7632(4)	608.79(8)
0.372(6)	11.3762(3)	14.0962(9)	3.7599(4)	602.93(7)
1.083(7)	11.3074(3)	13.9692(8)	3.7526(3)	592.74(6)
1.642(7)	11.2590(4)	13.8852(10)	3.7471(4)	585.80(8)
2.092(8)	11.2234(4)	13.8231(11)	3.7423(4)	580.58(8)
2.910(10)	11.1623(27)	13.7207(81)	3.7340(28)	571.87(54)
3.739(11)	11.1053(7)	13.6214(20)	3.7254(7)	563.53(13)
4.546(12)	11.0544(5)	13.5447(15)	3.7174(6)	556.60(11)
5.113(10)	11.0217(4)	13.4955(12)	3.7118(5)	552.11(8)
5.727(11)	10.9871(4)	13.4425(11)	3.7060(4)	547.35(8)
6.591(15)	10.9408(5)	13.3734(14)	3.6983(6)	541.12(10)
7.465(12)	10.8984(5)	13.3101(14)	3.6906(6)	535.34(10)
8.046(12)	10.8701(4)	13.2690(13)	3.6855(5)	531.58(9)

Standard deviations of the last digits are in parentheses.

TABLE 2. COEFFICIENTS RESULTING FROM THE FITS USING A THIRD-ORDER BIRCH–MURNAGHAN EQUATION OF STATE FOR UNIT-CELL PARAMETERS AND VOLUME

a_0	11.4162(3) Å	c_0	3.7638(3) Å
K_0	34.9(2) GPa	K_0	117(2) GPa
K'	6.23(8)	K'	2.5(6)
b_0	14.1709(9) Å	V_0	608.78(7) Å^3
K_0	22.1(2) GPa	K_0	37.2(2) GPa
K'	6.32(9)	K'	7.0(1)

The high-pressure crystal structure of berthierite

The high-pressure crystal-structure data, consisting of the refinements details, atom coordinates, displacement parameters and interatomic distances, are reported in Table 4, 5 and 6. A table with the anisotropic displacement parameters, the tables of structure factors and the cif files are available from the Depository of Unpublished Data on the Mineralogical Association of Canada website [Berthierite CM50_201].

As Figure 1 shows, the structure contains three distinct cation positions; Fe^{2+} has an octahedral coordination, and the polyhedra share edges with the conjugate Sb1 and Sb2 coordination polyhedra. The Fe coordination octahedra also share edges among themselves and form chains along [001]. As shown in Figure 5, the Sb1 site is a bicapped trigonal prism with the cation surrounded by eight sulfur atoms with five short distances ranging, at ambient pressure, from 2.49(1) Å to 2.983(3) Å, two additional sulfur atoms (S1) at 3.52(1) Å, and one additional sulfur atom (S2) at 3.606(7) Å. The Sb2 site is enclosed by a lying monocapped slightly distorted trigonal prism with, as for Sb1, five shorter bond-distances [2.438(9) – 3.208(6) Å] and two very long distances, 3.445(7) and 4.26(1) Å, respectively. The mesh of the Fe–S bonds and short Sb–S bonds forms rods parallel to [001], as seen on Figure 4. On the same figure, one can see that two Fe atoms from such a rod are bonded in addition to the ending S atoms of the two adjacent rods, and in this way limit the "LEP micelles" in the structure, the spaces with increased Sb–S bond lengths influenced by the LEP of Sb atoms.

Figure 6 shows the evolution of the bond lengths with pressure for the Fe, Sb1 and Sb2 coordination polyhedra. An analysis of the bond distances of Fe (Fig. 6a) shows that the Fe–S bonding distances undergo a shortening of about 4%. The exceptions are the medium to long Fe–S1 distances, which show only around 2% shortening. Whereas the longest (Fe–S4) bonds contract linearly over the whole range, the two shortest apical

TABLE 3. BULK MODULUS AND ITS FIRST DERIVATIVE FOR BERTHIERITE AND GALENOBISMUTITE AND THEIR RESPECTIVE COMPONENT SULFIDES

Compound	K_0 (GPa)	K'	Reference
$FeSb_2S_4$	37.2(2)	7.0(1)	This study
FeS	82(7)	-5(4)	King & Prewitt (1982)
Sb_2S_3	26.9(14)	7.9(1)	Lundegaard *et al.* (2003)
$PbBi_2S_4$	43.9(7)	6.9(3)	Olsen *et al.* (2007)
PbS	51.0(1.2)	4.3(9)	Knorr *et al.* (2003)
Bi_2S_3	36.6(15)	6.4(5)	Lundegaard *et al.* (2005)

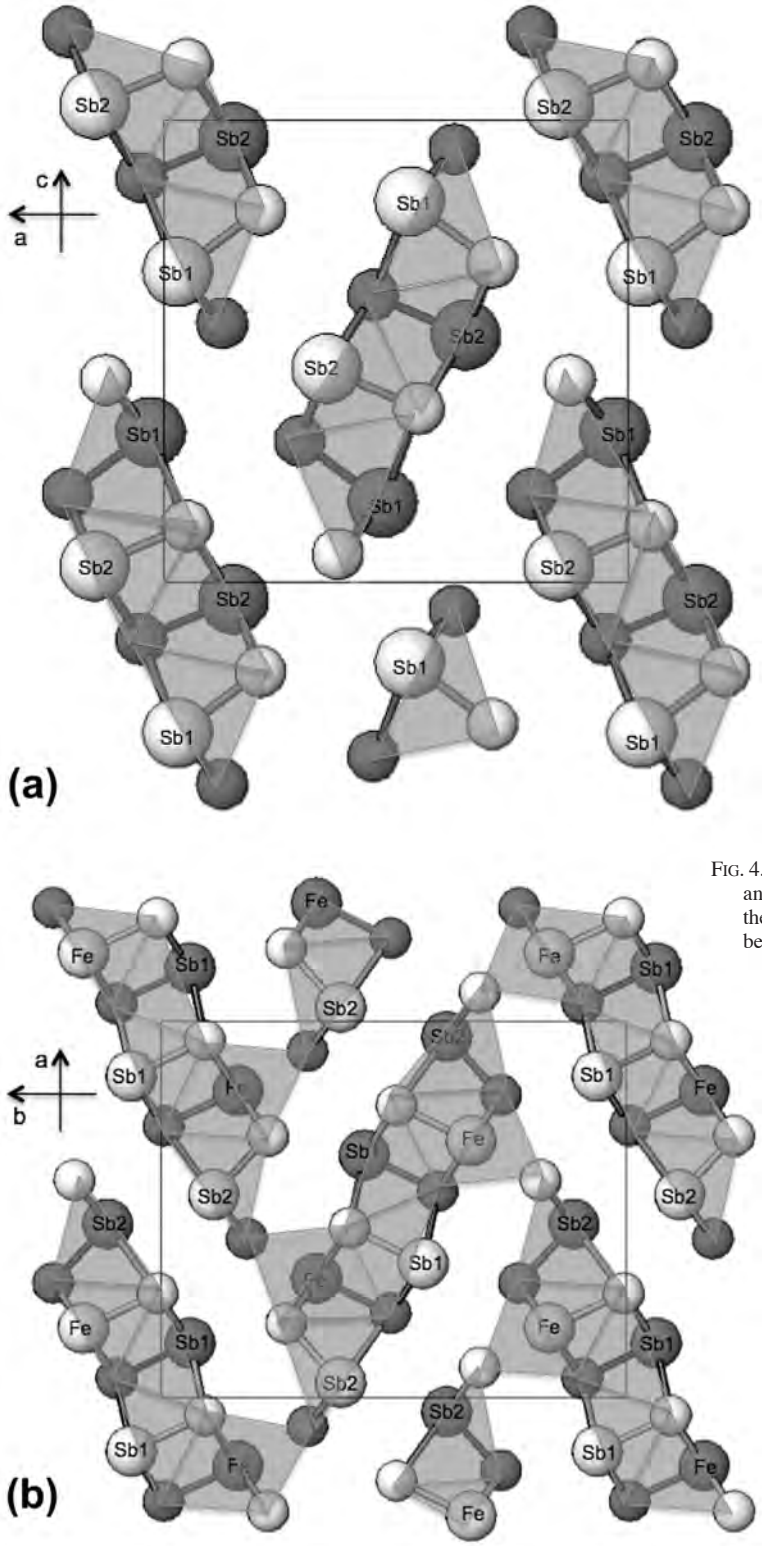


FIG. 4. Tightly bonded structural rods (grey) and intervening LEP spaces (white) in the crystal structures of a) stibnite and b) berthierite.

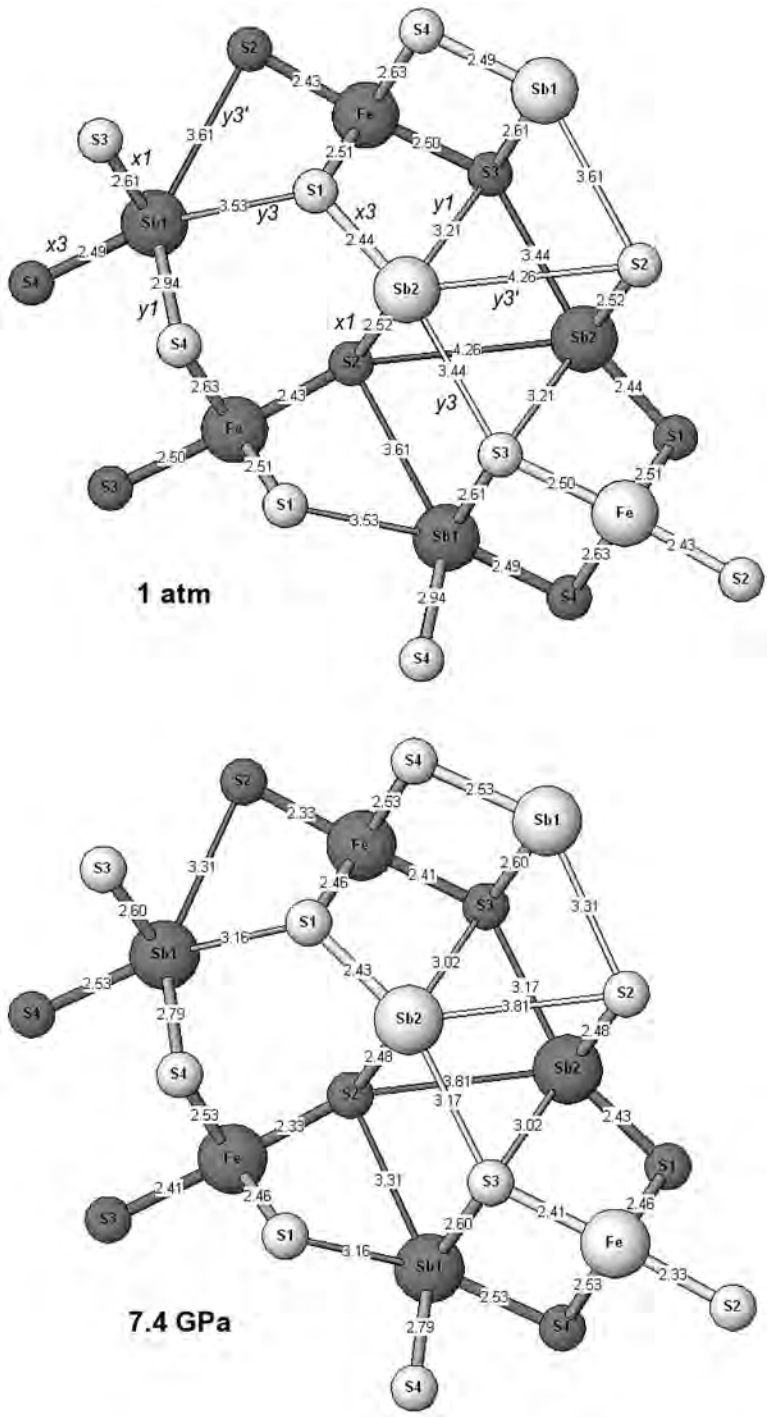


FIG. 5. Details of the Fe and Sb coordinations in the crystal structure of berthierite at 1 atm and 7.4 GPa. The labels *x* and *y* indicate short and respectively longer opposing bonds on Sb atoms.

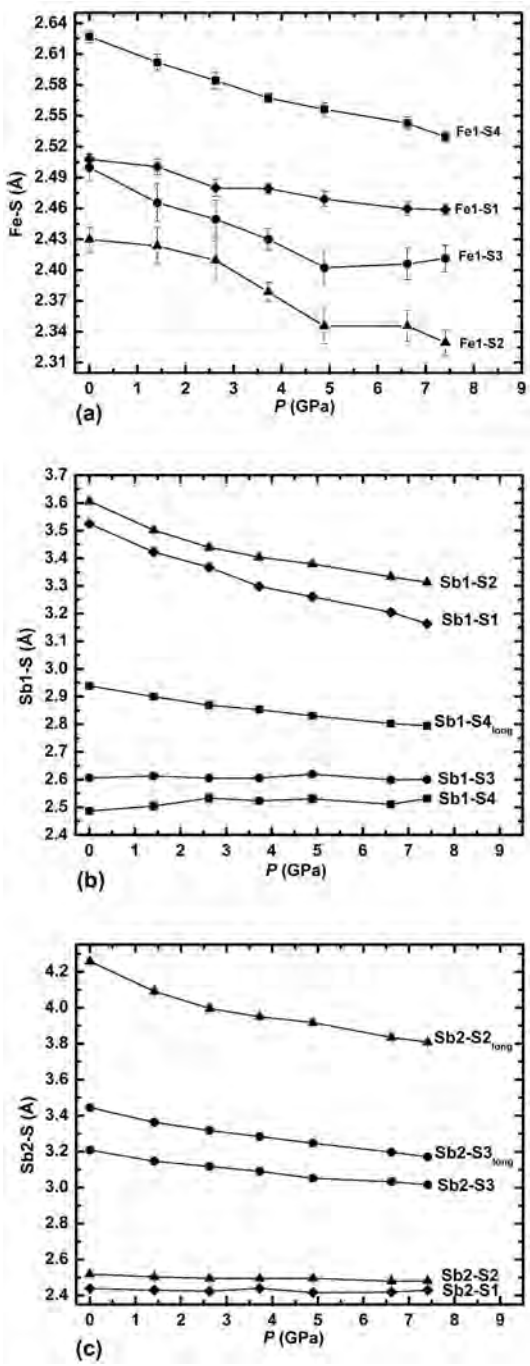


FIG. 6. Evolution of the individual bond-lengths as a function of pressure for Fe (a), Sb1 (b) and Sb2 (c) sites of berthierite.

bonds (Fe–S2 and Fe–S3) contract more quickly at the beginning, but then stabilize their lengths at about 5 GPa.

In Figure 6b and 6c, the bond distances for the Sb1 and Sb2 sites are shown as a function of pressure. As Figure 5 shows, the bonds appear in pairs consisting of a short (x_n) and an opposing long (y_n) Sb–S distance. The bond pairs called "out of plane" (x_3y_3 and x_3y_3') consist of the apical short bond of the square coordination pyramids SbS_5, with the short Sb–S bonds and one or more opposing long distance(s) below the base of the pyramid. The (x_1y_1) and (x_2y_2) bond pairs, called "in plane", lie in the square base of the SbS_5 pyramid (Berlepsch *et al.* 2001). The increase in the long Sb–S distance follows the decrease of the opposing bond-length along a hyperbolic trajectory, in agreement with the interdependence of the opposing bond-lengths typical of LEP elements such as As^{3+}, Sb^{3+} and Bi^{3+} (Berlepsch *et al.* 2001). In the case of high-pressure structures, the hyperbolic trend is still valid (Lundegaard *et al.* 2003), although the short Sb–S bonds tend to remain constant rather than to increase, as a result of the compression. The high-pressure evolution of the Sb–S distances is controlled by the LEP position (indicated by the centroid of coordination) which, at increasing pressure, is moving closer to the center of the atom, leading to a more symmetrical coordination of the Sb^{3+} atoms as a result (Lundegaard *et al.* 2005). As a consequence of this, the activity of the LEP appears to be lower at greater pressure. In turn, the other sulfur atoms, tightly bonded to Sb^{3+}, now become more strongly influenced by LEP, in some cases even producing a stretching of the short Sb–S bonds. In the case of berthierite, the Sb1–S1 (y_3' pair component) distance undergoes the greatest shortening, by 10.24%, whereas Sb1–S2 (y_3) experiences up to 8.14% contraction. The "out of plane" x_3 (S4) component of Sb1 is lengthened by 1.82%. The Sb2–S bond-distance compression is comparable to that of Sb1, as the longest bond-distance with S2 (y_3' pair component) is shortening by up to 10.55%, and $Sb2–S3_{long}$ (y_3), by 7.96%. In this case, the opposing x_3 component remains constant as a function of pressure. The "in plane" (y_1, y_2) distances for Sb1 and Sb2 sites undergo a similar shortening by 5–6%, whereas the respective short distances (x_1, x_2) remain almost unchanged.

COMPARISON OF THE HIGH-PRESSURE BEHAVIORS OF BERTHIERITE AND STIBNITE

In order to understand the effect of Fe on the deformation mechanism of berthierite, we present a comparison between our results with those obtained for stibnite (Lundegaard *et al.* 2003), a meneghinite homologue with composition Sb_2S_3. Similar to berthierite, the crystal structure of stibnite consists of tightly bonded Sb_4S_6 rods, with each Sb atom bonded to three to five S

TABLE 4. STRUCTURE-REFINEMENT DETAILS FOR BERTHIERITE

P (GPa)	0	1.41	2.63	3.72	4.89	6.62	7.41
a (Å)	11.4164(3)	11.2796(4)	11.1825(4)	11.1063(7)	11.0340(4)	10.9404(4)	10.9015(5)
b (Å)	14.1705(9)	13.9181(10)	13.7530(11)	13.6291(15)	13.5152(12)	13.3719(11)	13.3136(14)
c (Å)	3.7632(4)	3.7483(4)	3.7359(4)	3.7249(7)	3.7136(5)	3.6973(4)	3.6900(6)
V (Å^3)	608.80(8)	588.45(8)	574.55(8)	563.83(13)	553.80(9)	540.89(8)	535.56(11)
Range of *hkl*	-15 < *h* < 15 -6 < *k* < 6 -5 < *l* < 5	-14 < *h* < 15 -5 < *k* < 5 -5 < *l* < 5	-15 < *h* < 14 -5 < *k* < 5 -5 < *l* < 5	-15 < *h* < 14 -7 < *k* < 7 -5 < *l* < 5	-14 < *h* < 14 -4 < *k* < 5 -5 < *l* < 5	-14 < *h* < 14 -6 < *k* < 6 -5 < *l* < 4	-14 < *h* < 15 -6 < *k* < 6 -5 < *l* < 5
Unique reflections	344	290	290	372	258	300	322
Observed reflections [a]	291	244	246	304	219	251	272
2θ	59.7	59.4	59.4	59.4	60.1	59.3	59.4
R_{int}	9.0	12.0	12.3	17.6	12.9	7.8	6.9
R_1 (obs.)	5.3	6.3	6.5	6.4	5.1	6.0	4.4
wR_2 (obs.)	8.1	10.1	13.7	6.4	8.3	11.4	6.9
GooF	1.2	1.2	1.3	1.2	1.3	1.2	1.2
R.P.	32	32	23	32	32	23	32

Note: the data at 3.72 GPa were measured during decompression. [a] Criterion for observed reflections is $|F_o| > 4\sigma$. R.P.: refined parameters.

TABLE 5. COORDINATES AND DISPLACEMENT PARAMETERS OF ATOMS IN BERTHIERITE

P (GPa)		0.0001	1.41	2.63	3.72	4.89	6.62	7.41
Fe	*x*	0.3167(2)	0.3166(2)	0.3169(3)	0.3172(2)	0.3172(2)	0.3174(2)	0.3176(2)
	y	0.3340(5)	0.3339(7)	0.3338(7)	0.3338(4)	0.3341(6)	0.3343(6)	0.3341(5)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	U_{eq}	0.014(3)	0.016(6)	0.0139(9)	0.014(2)	0.014(6)	0.0129(8)	0.014(3)
Sb1	*x*	0.14445(8)	0.1440(1)	0.1439(1)	0.1436(1)	0.14339(9)	0.1430(1)	0.14293(8)
	y	0.0631(2)	0.0668(3)	0.0694(4)	0.0715(2)	0.0736(3)	0.0754(3)	0.0769(3)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	U_{eq}	0.016(2)	0.013(3)	0.0164(6)	0.011(1)	0.011(3)	0.0135(6)	0.011(2)
Sb2	*x*	0.03889(8)	0.0387(1)	0.0389(1)	0.0388(1)	0.03891(9)	0.0392(1)	0.03937(8)
	y	0.3862(2)	0.3894(3)	0.3914(3)	0.3926(2)	0.3936(3)	0.3953(3)	0.3962(2)
	z	0.75	0.75	0.75	0.75	0.75	0.75	0.75
	U_{eq}	0.016(2)	0.016(3)	0.0128(6)	0.010(1)	0.011(2)	0.0117(5)	0.012(2)
S1	*x*	0.1957(3)	0.1941(4)	0.1948(3)	0.1950(3)	0.1944(4)	0.1944(4)	0.1945(3)
	y	0.2694(8)	0.268(1)	0.269(1)	0.2668(6)	0.268(1)	0.266(1)	0.2652(8)
	z	0.75	0.75	0.75	0.75	0.75	0.75	0.75
	U_{iso}	0.014(1)	0.012(1)	0.014(1)	0.0111(9)	0.012(1)	0.013(1)	0.0106(9)
S2	*x*	0.4218(3)	0.4203(4)	0.4198(4)	0.4193(4)	0.4194(4)	0.4194(4)	0.4194(3)
	y	0.1849(8)	0.181(1)	0.180(1)	0.1804(7)	0.182(1)	0.180(1)	0.1803(9)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	U_{iso}	0.0137(9)	0.015(1)	0.012(1)	0.011(1)	0.014(1)	0.013(1)	0.0104(9)
S3	*x*	0.2233(3)	0.2221(4)	0.2224(4)	0.2223(4)	0.2208(4)	0.2211(4)	0.2205(3)
	y	0.4935(8)	0.494(1)	0.494(1)	0.4945(7)	0.494(1)	0.496(1)	0.4968(9)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	U_{iso}	0.016(1)	0.013(1)	0.012(1)	0.010(1)	0.012(1)	0.012(1)	0.010(1)
S4	*x*	0.4507(3)	0.4511(4)	0.4522(5)	0.4515(4)	0.4520(4)	0.4520(4)	0.4519(3)
	y	0.4053(8)	0.404(1)	0.403(1)	0.4032(6)	0.403(1)	0.404(1)	0.4033(8)
	z	0.75	0.75	0.75	0.75	0.75	0.75	0.75
	U_{iso}	0.014(1)	0.014(1)	0.012(1)	0.012(1)	0.011(1)	0.011(1)	0.010(1)

atoms by short bonds, and with their LEP oriented into the space between the rods. As in berthierite, the two Sb positions are independent, with Sb1 at the margin of the Sb_4S_6 ribbon and Sb2 atoms placed around the center of the ribbon. Both are seven-fold-coordinated, with a lying monocapped trigonal prism at the Sb1 position and a standing monocapped trigonal prism at the Sb2 site. The Sb coordination prisms of stibnite resemble those in berthierite, with equivalences $Sb1_{btr} - Sb2_{sbn}$ and $Sb2_{btr} - Sb1_{sbn}$ (Fig. 4). As mentioned earlier and

as is visible in Figure 4, the main difference between the two structures comes from the role of the [FeS_6] coordination which, in berthierite, bridges the adjacent tightly bonded rods, borders LEP micelles, and puts limits on the rotation of the rods under compression.

The evolution of the relative volumes of polyhedra for berthierite and stibnite with pressure shows analogies of the Sb sites in these structures and the influence of Fe in berthierite (Fig. 7).

The IVTON program (Balić-Žunić & Vickovic 1996) was used to calculate the polyhedron volumes and distortion parameters based on the centroid of coordination (Balić-Žunić & Makovicky 1996). From a comparison of the polyhedron compressibilities (Fig. 7a), the following conclusions can be made.

The volumes decrease non-linearly as a function of pressure, and all show stiffening. From Figure 7a, the Fe site emerges as the least compressible site, but with two distinct, practically linear trends up to and above 5 GPa, respectively. The trends show that the compression after 5 GPa is significantly slower than the one at lower pressures.

At the beginning, the volume of polyhedron Sb2 in berthierite shows the most marked compression, overlapping perfectly with the $Sb1_{sbn}$ trend. This, however, changes at about 3 GPa, after which its compression slows down more than that of $Sb1_{sbn}$. At higher pressures, the two Sb coordination polyhedra in berthierite achieve the same degree of compression, unlike the Sb coordination polyhedra in stibnite, which continue to diverge. The relative variation in volume of Sb1 and Sb2 in berthierite is within one standard deviation, and their compression rate is very similar up to 7.41 GPa ($\Delta V_{Sb1btr} = 13.5\%$ and $\Delta V_{Sb2btr} = 13.4\%$). In stibnite, the resulting $\Delta V_{\%}$ up to 7.832 GPa are 11.3 and 15.7 for Sb2 and Sb1, respectively. The changes of the compressional trends of Sb coordination polyhedra in berthierite can be attributed to the change that the Fe coordination experiences at about 5 GPa.

Figures 7b, 7c and 7d show the change of the distortion parameters of the polyhedra in berthierite and stibnite as a function of pressure. As is typical for elements with LEP, the largest distortion is due to eccentricity of the Sb sites. If the LEP activity is quantified using the eccentricity parameter, the $Sb2_{btr}$ polyhedron shows a larger value than the rest of berthierite polyhedra and the stibnite sites. As expected for stable crystal structures (Balić-Žunić 2007), the eccentricity of Sb decreases as a function of pressure, but still at the highest pressure, the eccentricity is found to be above the values typical for elements without pairs of lone electrons, as exemplified by the value for the Fe coordination. The eccentricities of Sb in berthierite remain at higher values compared to those in stibnite. This is most probably due to the blocking influence of the Fe coordination on the inter-rod compression. The asphericity values for Sb in berthierite are much higher than those for stibnite at all pressures. The decrease of asphericity of the two Sb sites in berthierite is not linear and shows a "fast" trend up to about 2–3 GPa, especially for the Sb2 site. This

TABLE 6. SELECTED BOND-LENGTHS AND POLYHEDRON VOLUMES IN BERTHIERITE

Pressure (GPa)	0.0001	1.41	2.63	3.72	4.89	6.62	7.41
Fe-S2 [(i)]	2.430(12)	2.423(18)	2.409(18)	2.379(9)	2.348(17)	2.346(15)	2.329(12)
Fe-S3 [(i)]	2.500(13)	2.465(18)	2.449(18)	2.430(10)	2.404(18)	2.406(15)	2.411(13)
Fe-S1 [(i, ii)]	2.508(5)	2.500(8)	2.480(8)	2.479(4)	2.468(7)	2.460(7)	2.459(5)
Fe-S4 [(i, ii)]	2.627(6)	2.602(8)	2.584(8)	2.567(4)	2.555(7)	2.543(6)	2.529(5)
V	21.4(1)	21.0(1)	20.6(1)	20.20(8)	19.8(1)	19.6(1)	19.4(1)
Sb1-S4 [(iii)]	2.486(12)	2.504(16)	2.533(17)	2.524(8)	2.533(15)	2.511(13)	2.532(11)
Sb1-S3 [(ii, iv)]	2.606(5)	2.613(7)	2.605(7)	2.606(4)	2.619(7)	2.599(6)	2.600(5)
Sb1-S4 [(v, vi)]	2.938(3)	2.900(4)	2.870(4)	2.853(3)	2.829(3)	2.803(4)	2.795(3)
Sb1-S1 [(i, ii)]	3.524(10)	3.422(14)	3.367(15)	3.298(7)	3.262(14)	3.205(12)	3.163(9)
Sb1-S2 [(i)]	3.606(7)	3.501(9)	3.439(9)	3.404(6)	3.378(8)	3.332(8)	3.313(6)
V	46.6(2)	45.0(2)	43.8(3)	42.8(2)	42.3(3)	40.8(2)	40.4(2)
Sb2-S1 [(i)]	2.438(9)	2.429(13)	2.424(14)	2.439(7)	2.417(13)	2.418(12)	2.429(9)
Sb2-S2 [(v, vi)]	2.518(5)	2.504(7)	2.494(7)	2.494(4)	2.495(7)	2.479(6)	2.480(5)
Sb2-S3 [(i, vii)]	3.208(6)	3.146(9)	3.116(8)	3.090(5)	3.051(8)	3.032(7)	3.016(6)
Sb2-S3 [(viii)]	3.445(7)	3.363(9)	3.317(10)	3.283(6)	3.246(8)	3.196(8)	3.170(6)
Sb2-S2 [(ix)]	4.257(12)	4.090(17)	3.996(18)	3.950(9)	3.922(17)	3.834(14)	3.808(12)
V	38.2(1)	36.4(2)	35.4(2)	34.9(1)	34.2(2)	33.3(2)	33.0(1)

Symmetry codes: (i): x, y, z; (ii): x, y, z – 1; (iii): –x + 1/2, y – 1/2, z – 1/2; (iv): –x + 1/2, y – 1/2, z + 1/2; (v): x – 1/2, –y + 1/2, –z + 1/2; (vi): x – 1/2, –y + 1/2, –z + 3/2; (vii): x, y, z + 1; (viii): –x, –y + 1, –z + 1; (ix): –x + 1/2, y + 1/2, z + ½. Bond lengths are expressed in Å, and unit-cell volumes, in $Å^3$.

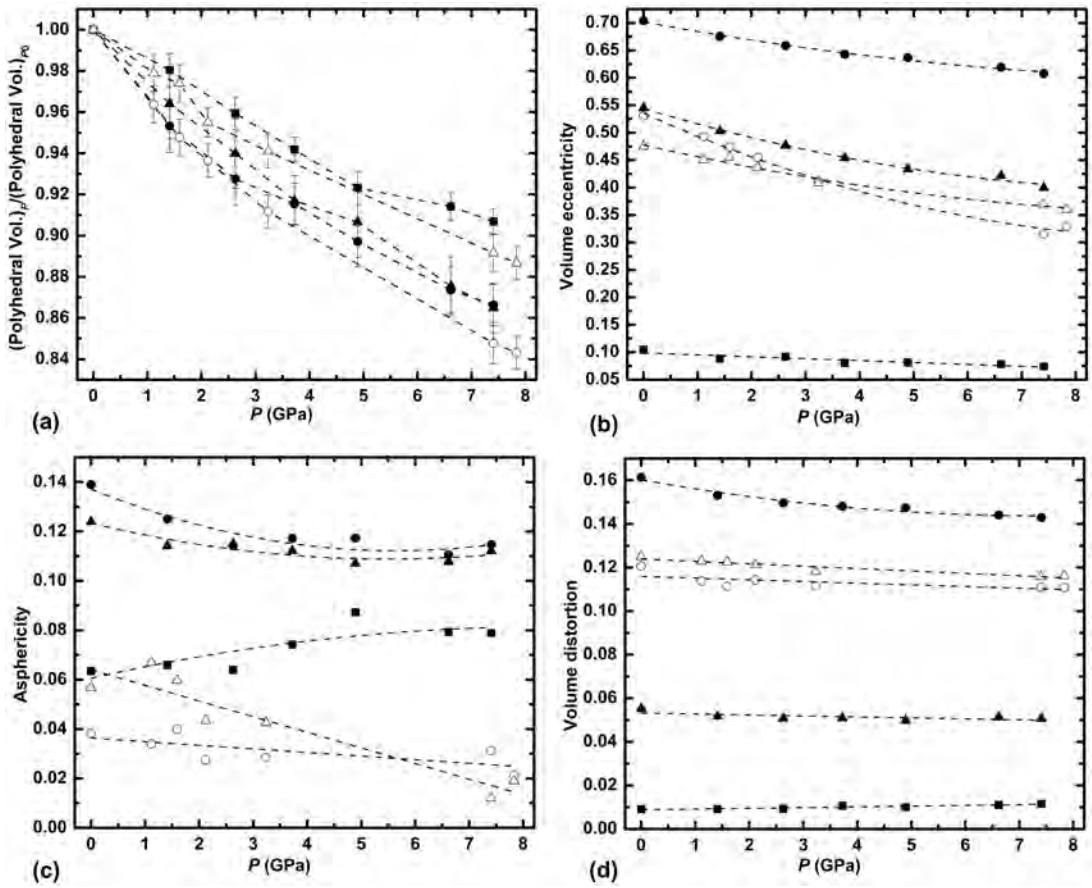


FIG. 7. Comparison of the coordination polyhedra of berthierite (black symbols) and stibnite (open symbols). Squares: Fe site; triangles: $Sb1_{btr}$ and $Sb2_{sbn}$; circles: $Sb2_{btr}$ and $Sb1_{sbn}$. Evolution as a function of pressure of: (a) relative compression of the polyhedron volume, (b) eccentricity, (c) asphericity and (d) volume distortion.

decrease is followed by a rapid leveling off, indicating a kind of equilibrium condition for the Sb sites at higher pressure. At the same pressure, the asphericity of iron noticeably increases owing to the strong dissymmetrization undergone up to about 5 GPa, after which it slowly levels off. Finally, the volume-distortion parameter is the one that is the least influenced by the compression of the structure, remaining almost constant throughout the entire measured range of pressure for both berthierite and stibnite. The only visible decrease, expressing its initial large value, is observed for the coordination polyhedron of $Sb2_{btr}$, which also in this respect is the most irregular of all.

MODULES IN THE BERTHIERITE AND STIBNITE STRUCTURES

Following the same approach applied to stibnite and bismuthinite by Lundegaard *et al*. (2003, 2005), the unit-cell space can be divided into tightly bonded rods and the rest of the space influenced by LEP. In the case of berthierite, the section areas of tightly bonded rods comprise eight triangles per ribbon with vertices in the S sites (Fig. 4). The sum of the area of two ribbons gives the area of the tightly bonded rods per unit cell; the rest is the LEP space. This separation allows us to separate the bulk effect of pressure on the two qualitatively different bonding environments.

As expected, the LEP space accommodates most of the compression, both in berthierite and in stibnite (Fig. 8a). The LEP areas are almost equal in the two structures, but the tightly bonded rod areas are much

larger in berthierite. As the compression is mostly accommodated by the LEP spaces, this gives a larger compressional potential to stibnite, as reflected in significantly lower K_{T0}. In both structures, the A_{rod}:A_{LEP} ratio increases with pressure but not linearly, which is primarily due to a decreased rate of LEP compression (Fig. 8b). In berthierite, an important change in trend also is observed between 3 to 5 GPa. For stibnite, the situation is not so clear owing to a large gap in observations between 3.5 and 7 GPa.

Relationship of Berthierite to the $CaFe_2O_4$ Structural Family

As stated earlier, berthierite is isopointal with galenobismutite ($PbBi_2S_4$; Pinto *et al*. 2005, Olsen *et al*. 2007). They both are isopointal with the broad structural family of $CaFe_2O_4$ (CFO; Decker & Kasper 1957). Olsen *et al*. (2007) have shown that among the known members of the family, it is $PbSc_2S_4$ (Shemet *et al*. 2006) that has the most regular archetypal structure (Fig. 9a), with two octahedral (Sc) sites and one bicapped trigonal prismatic site (Pb). The comparison to this structure can therefore be used to estimate the distortion from the ideal structure-type.

Galenobismutite shows a relatively large distortion with respect to the idealized CFO-type structure (Fig. 9b). The coordination of the Bi2, equivalent to Sc1, is changed from a fairly regular octahedral coordination to a lying monocapped trigonal prism by an opposite translation of the atoms in the two adjacent Bi2 coordination polyhedra parallel to the equatorial plane of the octahedra. This movement of the central atomic groups in Figure 9b influences the other coordination polyhedra as well, so that the coordination polyhedron of Pb becomes transitional between a bicapped and a monocapped standing trigonal prism, by the displacement of the S4 atom away from the Pb atom. At the same time, the coordination polyhedron of Bi1, which corresponds to almost perfectly octahedrally coordinated Sc2 in $PbSc_2S_4$, is a distorted octahedron in galenobismutite with one significantly elongate bond (to the apical S1).

The crystal structure of berthierite presents a continuation of the distortion represented by the galenobismutite structure. In this case, the discrepancy from the archetypal motif represented by $PbSc_2S_4$ produces even a recombination of some atomic bonds through a significantly larger relative displacement of the atoms (Fig. 9c). The opposite movement of the central atomic groups in Figure 9 goes one step beyond the situation in galenobismutite, and in berthierite the Fe atoms, equivalent to Bi2 in galenobismutite, now face S3 atoms, equivalent to S1 in galenobismutite, and break the bond to the S4 atoms, equivalent to S3 in galenobismutite. The coordination pair represented by Sc1, Sc1 in $PbSc_2S_4$ and Bi2, Bi2 in galenobismutite is now separated, and a new octahedral coordination of the sites here occupied by Fe is achieved by the break of one bond and the establishment of another one. The structure of galenobismutite clearly represents a transition between the structures of $PbSc_2S_4$ and berthierite, in which the bonding to the two alternative S atoms for the octahedra of Sc1 and Fe is simultaneously present in a transitional coordination with the coordination number 7. The increased movements of atoms in berthierite compared to $PbSc_2S_4$ and galenobismutite affect also the other coordination polyhedra, so that the bonding in Sb1, equivalent to Pb in both $PbSc_2S_4$ and galenobismutite, also switches one of the capping atoms. The distance to the sulfur atom, which has been

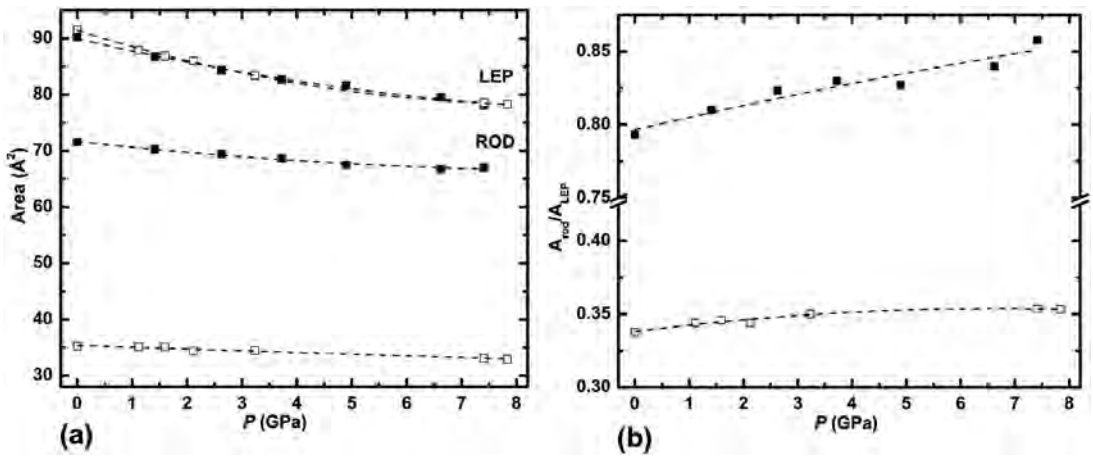
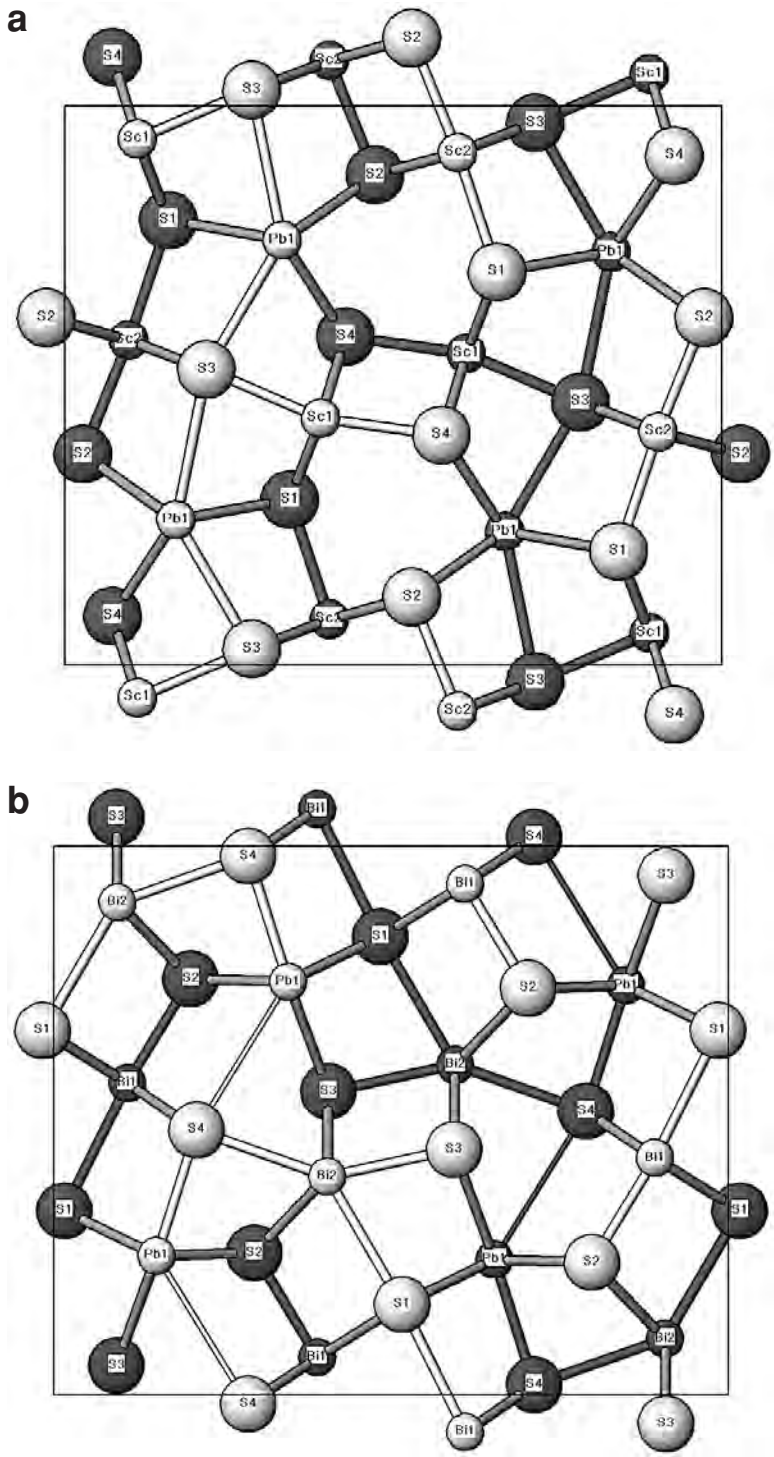


Fig. 8. (a) Calculated LEP areas and rod areas from the berthierite (black symbols) and stibnite (open symbols). (b) Ratio of the rod area to the LEP area for berthierite and stibnite.


a
S4
S2
Sc2
S3
Sc1
Sc1
S3
S4
Sc1
Sc2
S2
S1
Pb1
S1
Pb1
S2
S2
Sc2
S4
Sc1
S2
S3
S3
Sc1
S4
Sc2
S2
S2
S1
Pb1
Pb1
S1
S4
Sc2
S2
Sc1
S3
S3
Sc1
Sc2
S4
b
S3
Bi1
S4
S4
S3
Bi1
Bi2
S1
S2
Pb1
S2
Pb1
S1
S1
Bi1
S3
Bi2
S4
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S3
S3
Bi2
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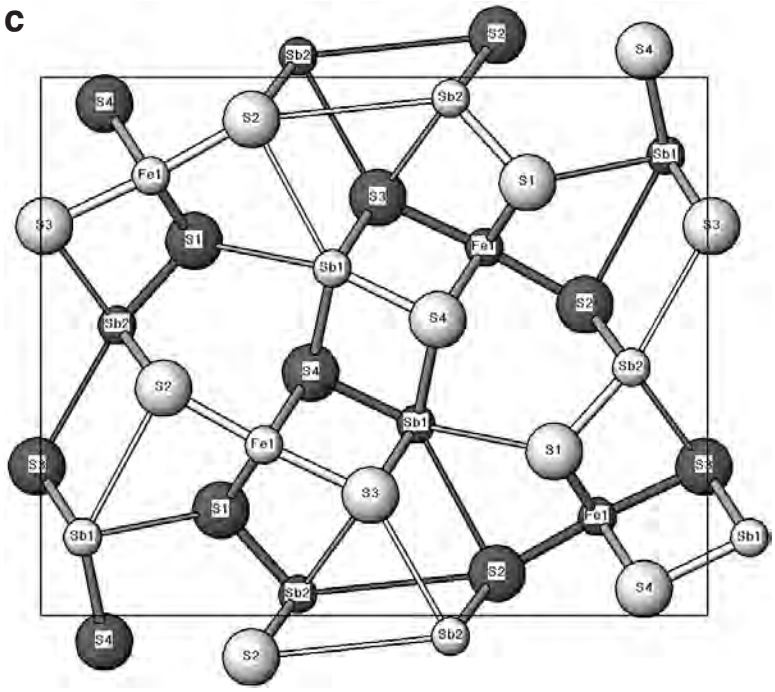

FIG. 9. Relation between the CFO structure type represented by $PbSc_2S_4$ (a), galenobismutite (b) and berthierite (c) structures. One can appreciate basically the same crystallographic set of sites, but with large relative lateral movements, with the consequent changes in the bonding scheme.

elongated in galenobismutite (S2 in berthierite, S4 in galenobismutite) is now increased beyond the coordination sphere, but at the same time, a new bond is established to the approaching S4 atom (equivalent to S3 in galenobismutite). The Sb2 coordination, equivalent to Bi1 in galenobismutite, is now largely distorted, with the coordination number increased to 7 by further movements compared to galenobismutite. All these additional aspects are in agreement with the transitional position of galenobismutite between the structures of $PbSc_2S_4$ and berthierite.

The difference in the orientation of short bonds in berthierite and galenobismutite produces different orientations of LEP with a more heterogeneous orientation in galenobismutite than in berthierite. Although the formation of the LEP micelles in berthierite resembles more the situation in stibnite, a comparison of the compressional characteristics shows more resemblance to galenobismutite, owing to basically the same structure-type and a closer similarity in the coordination characteristics. Figure 10 shows the volume compressions and distortion parameters for berthierite and galenobismutite and should be compared to Figure 7. The compressibilities of the coordination polyhedra with the same coordination numbers in the two structures are very much the same (pairs Fe–Bi1, Sb1–Pb and Sb2–Bi2). There are small differences in the trends. The compressibility of the Fe coordination polyhedron is larger at lower than at higher pressures, as mentioned earlier, whereas the Bi1 site shows a closer to linear behavior. As Fe compresses more rapidly up to 5 GPa and then slower than Bi1, the two coordination polyhedra achieve approximately the same compression at 8–9 GPa. Both Sb1 and Pb show a very similar behavior through all pressures, contrary to the Sb2 in stibnite, which is significantly less compressible. Polyhedron $Sb2_{btr}$, which is less compressible than its counterpart in stibnite (Sb1), is generally more compressible than Bi2 in galenobismutite. Eccentricities are significantly lower in galenobismutite, apart from Fe, which is the only cation without LEP. Otherwise, the trends under compression are very similar. The octahedrally coordinated Bi1 in galenobismutite remains almost unchanged in its eccentricity like Fe in berthierite, whereas the two other coordination polyhedra show a compression conformable to that of the two Sb sites in berthierite. In this way, the basic coordination characteristics and differences between the two structures remain largely

unchanged throughout the pressure range investigated. Note that the site with the coordination number 7 in berthierite (Sb2) has a larger eccentricity than the site with the coordination number 8 (Sb1), whereas it is the opposite in galenobismutite.

Although the eccentricities in stibnite are generally large and approach that of the Sb1 in berthierite, the trends under compression are different. Atom Sb2 in stibnite decreases its eccentricity more slowly and approaches that of $Sb1_{btr}$ at the highest pressures. On the other hand, $Sb2_{sbn}$ starts with the same eccentricity, but it decreases more rapidly and results in the least eccentric Sb site at the highest pressures. Note that the Pb site in galenobismutite is the most aspheric of all coordination polyhedra, whereas the Bi1 octahedron from the same structure appears almost perfectly spherical. The asphericities of the Sb sites in berthierite assume values midway between those of Pb and Bi sites in galenobismutite. The Bi2 site shows a constant decrease in this distortion parameter, contrary to the crystallographically equivalent Fe.

The volume distortion can be related to the elongation or contraction of the polyhedron and can be used for the estimation of the coordination type (Makovicky & Balić-Žunić 1998). The values, calculated with the program IVTON, are related to the coordination type with the highest effective volume given the same coordination number and polyhedron size. For the coordination numbers present in berthierite and galenobismutite, the maximum-volume polyhedra are octahedron (CN6), pentagonal bipyramid (CN7) and bisdisphenoid (CN8). As can be seen from Figure 10d, the two octahedral coordinations (Fe and Bi1) show only a very small discrepancy from an ideal octahedron. The CN8 sites (Sb1 and Pb) show practically the same values, which correspond best to the square antiprism. Compared to

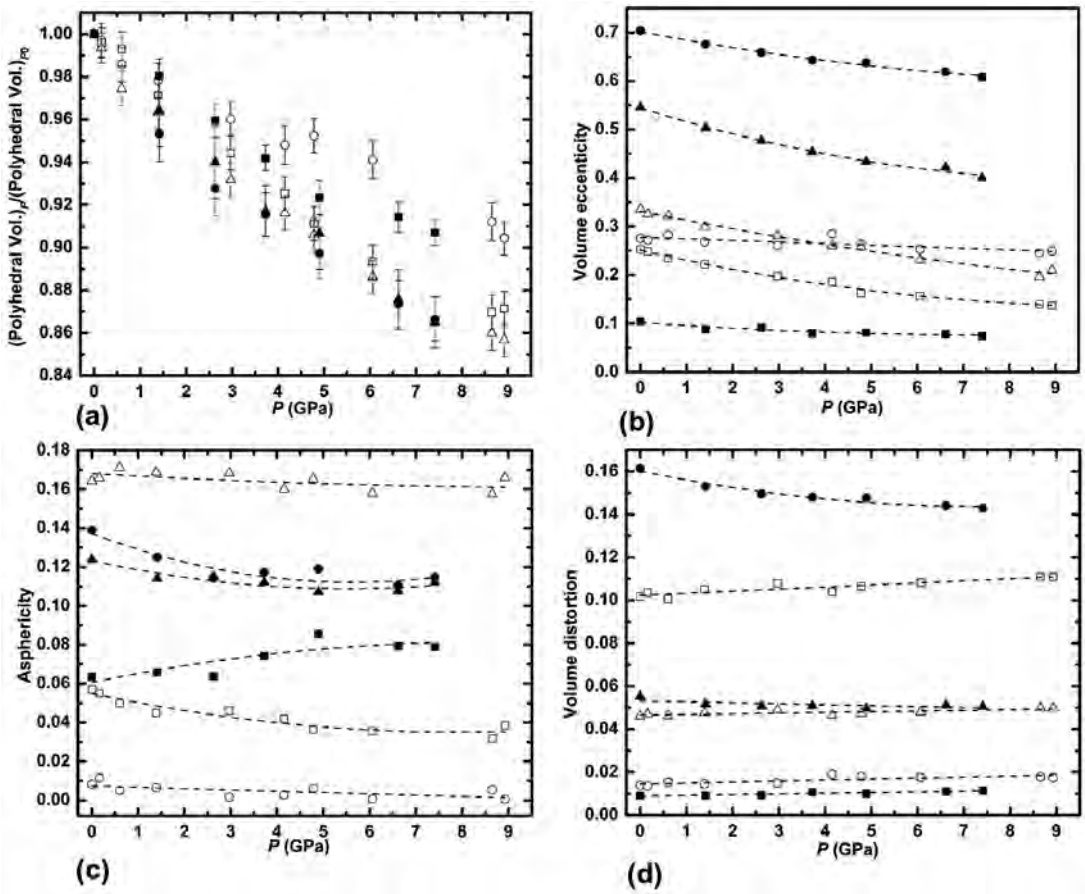

FIG. 10. Comparison of coordination polyhedra in berthierite (black symbols) with galenobismutite (open symbols). Evolution of (a) relative polyhedron volume, (b) eccentricity, (c) asphericity and (d) volume distortion as a function of pressure. (Squares: Fe and Bi2; triangles: Sb1 and Pb; circles: Sb2 and Bi1).

a bisdisphenoid, an Archimedean square antiprism of the same diameter has a smaller volume, which gives a value of volume distortion of 0.053 (Makovicky & Balić-Žunić 1998). The sites with CN7 show the most interesting behavior. At atmospheric pressure, they have largely different distortions: Sb2 in berthierite has a value that best corresponds to that of a monocapped trigonal prism (volume distortion 0.163; Makovicky & Balić-Žunić 1998), whereas Bi2 in galenobismutite has a significantly lower value. With increasing pressures, the distortions behave differently also. Site $Sb2_{btr}$ lowers the volume distortion, whereas Bi2 increases it. In this way, they both converge toward 12–13% distortion, which is close to the value characteristic of the so-called split octahedron (volume distortion 0.133; Makovicky & Balić-Žunić 1998). The situation in stibnite is quite different. Both Sb coordination polyhedra in this structure show similar and relatively stable volume-distortions (Fig. 7d), resembling the one of Bi2 from galenobismutite.

Conclusions

The high-pressure single-crystal diffraction study of berthierite, $FeSb_2S_4$, presented here is the first detailed study of a crystal structure of a sulfosalt of Sb under compression.

No evidence of a phase transition has been found up to about 8 GPa. The bulk modulus (K_{T0}) is somewhat smaller but comparable to that of galenobismutite, $PbBi_2S_4$, and significantly larger than that of stibnite, Sb_2S_3. The LEP stereochemical activity is expected to be higher for Sb than for Bi, as it generally diminishes with increasing atomic number of the metal within a group (Grzechnik 2007). Owing to this general systematic decrease, the unit cell containing Sb atoms should have a softer response to compression than one containing Bi. On the other hand, the presence of Fe in berthierite and its specific structural role seem to increase the value of its bulk modulus compared to that of stibnite.

Like in all other structures with LEP so far investigated, the compression at low to medium pressures is mainly achieved through shortening of the long bonds influenced by LEP. Their opposing short bonds do not show a significant shortening with pressure, and some may even increase, testifying for the movement of the LEP toward a central position in the atom as a function of pressure.

The closer similarity of EoS parameters of berthierite to those of galenobismutite than to those of stibnite is also connected to a closer resemblance in the evolution of the crystal-structure parameters with pressure. Although the distribution of bonds and the rod-based structure of berthierite resemble the general structural topology of stibnite, the kinship with galenobismutite through the affiliation to the same crystallographic structure-type and the existence of the same coordination types in the structure seem to be more important for the compressional characteristics. By means of the geometrical analysis of the compression of tightly bonded rod areas and LEP areas, we can confirm that, as for other structures with LEP, the dissymmetrization effect due to the pair of lone electrons decreases with pressure. The response of the LEP to compression seems to be the main reason for the stiffening of the crystal structure in the range investigated and a high *K*' value. Moreover, the development of A_{rod}:A_{LEP} experiences a substantial change in the pressure range of 3–5 GPa. A change in this pressure range is observed also in the other structural parameters and can be directly related to the behavior of the Fe–S coordination sphere.

The main peculiarity of berthierite is the behavior of Fe coordination. Like the octahedral coordination of Bi1 in galenobismutite, it is the stiffest one in the structure, and both show a similar contraction in the range investigated. However, the coordination of Fe shows two distinct trends, below and above 4–5 GPa, respectively. It undergoes a dissymmetrization, akin to a Jahn–Teller effect, which reaches a maximum at about 5 GPa. At higher pressures, the coordination polyhedron shows a stiffer response to compression, and the Jahn–Teller distortion remains at the level achieved.

If the evolution of unit-cell parameters *a* and *b* is taken into account, it is noteworthy that beyond approximately 4 GPa, a slight change of slope is evident (Fig. 2a). This indicates a pronounced stiffening of the crystal structure in the plane perpendicular to the **c** axis beyond about 4 GPa, a behavior that could not be accurately fitted by the standard functions applied. The **c** axis itself compresses linearly throughout the investigated range. The observed effect is most probably related to the behavior of Fe and influenced by the change in the characteristics of its coordination.

Atom Fe^{2+}, with its d^6 configuration, can show a Jahn–Teller effect in a relatively weak crystal-field in which the high-spin configuration can be attained, which would remove the degeneracy of the unequally filled t_{2g} orbitals. Indeed, in the crystal structure of jamesonite ($FePb_4Sb_6S_{14}$; Niizeki & Buerger 1957), an equally distorted octahedral coordination of Fe^{2+} can be found. It is intriguing that in the isotypic structure of benavidesite ($Mn^{2+}Pb_4Sb_6S_{14}$; Léone *et al*. 2003), Mn^{2+} also shows a distorted coordination, although d^5 configurations, contrary to d^6, are expected to show the Jahn–Teller effect in the low-spin and not the high-spin configurations. The increase in the distortion of the Fe site with pressure in berthierite, which, however, reaches a maximum at a pressure of about 5 GPa, is an interesting phenomenon and obviously one that has a pronounced influence on the total structural development. It will be interesting to study the high-pressure behavior of the other members of the berthierite isotypic series: garavellite ($FeSbBiS_4$; Strunz & Nickel 2001,

Bindi & Menchetti 2005) and clerite ($MnSb_2S_4$; Murzin *et al*. 1996).

Acknowledgements

We dedicate this article to Emil Makovicky on the occasion of his "official" retirement. To an experienced reader, Emil's influence in this work is clearly visible, but what may not be obvious is that we discussed all the details with him, gaining an indispensable help in writing the manuscript. The team responsible for this work illustrates well the long-lasting influence that his science has had on mineralogical research, comprising a young researcher just getting some of the most important insights into the rules of crystal structures from him, an established researcher gaining from contacts with Emil the revelations about the fantastic world of sulfosalts, and one of Emil's long-time collaborators who is deeply indebted to him for many things, but probably mostly for the opportunity to share in discoveries of some of the most beautiful patterns in the nature.

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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0284P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0000(8)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          258
_refine_ls_number_parameters      32
_refine_ls_number_restraints      0
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S2 S 0.4194(4) 0.1818(12) 0.2500 0.0145(11) Uiso 1 2 d S . .
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_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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;
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_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
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_diffrn_detector_area_resol_mean  ?
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_diffrn_reflns_number             1759
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_diffrn_reflns_av_sigmaI/netI     0.0555
_diffrn_reflns_limit_h_min        -14
_diffrn_reflns_limit_h_max        14
_diffrn_reflns_limit_k_min        -6
_diffrn_reflns_limit_k_max        6
_diffrn_reflns_limit_l_min        -5
_diffrn_reflns_limit_l_max        4
_diffrn_reflns_theta_min          3.72
_diffrn_reflns_theta_max          29.63
_reflns_number_total              300
_reflns_number_gt                 251
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        ?
_computing_data_reduction         ?
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?
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;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0601P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0029(9)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          300
_refine_ls_number_parameters      23
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0761
_refine_ls_R_factor_gt            0.0599
_refine_ls_wR_factor_ref          0.1142
_refine_ls_wR_factor_gt           0.1070
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_refine_ls_restrained_S_all       1.180
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_refine_ls_shift/su_mean          0.000

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S1 S 0.1944(4) 0.2666(11) 0.7500 0.0131(12) Uiso 1 2 d S . .
S2 S 0.4194(4) 0.1800(10) 0.2500 0.0127(11) Uiso 1 2 d S . .
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_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Fe S1 2.460(7) . ?
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Fe S4 2.543(6) 1_554 ?
Fe Sb2 3.654(3) 1_554 ?
Fe Sb2 3.654(3) . ?
Fe Fe 3.6973(4) 1_556 ?
Fe Fe 3.6973(4) 1_554 ?
Fe Sb1 3.742(8) 7_666 ?
Fe Sb1 3.742(8) 7_665 ?
Fe Sb1 3.761(4) 3 ?
Fe Sb1 3.953(8) . ?
Fe S4 4.309(13) 5_666 ?
Fe Sb2 4.327(6) 3 ?
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Fe S2 4.358(5) 3_455 ?
Fe S2 4.379(8) 1_554 ?
Fe S2 4.379(8) 1_556 ?
Fe S3 4.411(8) 1_556 ?
Fe S3 4.411(8) 1_554 ?
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Fe S1 4.716(6) 3 ?
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Fe Sb1 5.274(3) 3_554 ?
Fe Sb2 5.319(6) 5_566 ?
Fe Sb1 5.413(6) 1_554 ?
Fe Sb1 5.413(6) 1_556 ?
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Fe S2 5.613(14) 7_665 ?
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S3 Fe Sb1 43.63(17) . 7_665 ?
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S4 Fe Sb2 104.3(2) 1_554 3_556 ?
Sb2 Fe Sb2 147.3(2) 1_554 3_556 ?
Sb2 Fe Sb2 114.16(10) . 3_556 ?
Fe Fe Sb2 64.71(4) 1_556 3_556 ?
Fe Fe Sb2 115.29(4) 1_554 3_556 ?
Sb1 Fe Sb2 109.59(6) 7_666 3_556 ?
Sb1 Fe Sb2 139.24(9) 7_665 3_556 ?
Sb1 Fe Sb2 72.36(9) 3 3_556 ?
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Sb2 Fe S2 33.08(12) 3_556 1_556 ?
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S3 Fe S3 56.95(17) . 1_554 ?
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Sb'  'Sb'  -0.5866   1.5461
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    ?

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 'x+1/2, -y+1/2, -z+1/2'
 '-x+1/2, y+1/2, -z'
 '-x, -y, -z'
 'x, y, -z-1/2'
 '-x-1/2, y-1/2, z-1/2'
 'x-1/2, -y-1/2, z'

_cell_length_a                    10.9015(5)
_cell_length_b                    13.3136(14)
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_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
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_exptl_absorpt_process_details    Absorb(Angel,2004)

_exptl_special_details
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_reflns_number_gt                 272
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_computing_molecular_graphics     ?
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0020(5)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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_refine_ls_number_parameters      32
_refine_ls_number_restraints      0
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_refine_ls_wR_factor_ref          0.0741
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 _atom_site_aniso_U_12
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Fe S1 2.459(5) . ?
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Fe S4 2.529(5) 1_554 ?
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Fe Sb2 3.645(3) . ?
Fe Fe 3.6900(6) 1_556 ?
Fe Fe 3.6900(6) 1_554 ?
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Fe Sb1 3.747(6) 7_666 ?
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Fe S4 4.306(11) 5_666 ?
Fe Sb2 4.319(5) 3 ?
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Fe S2 4.364(7) 1_556 ?
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Sb1 S4 Sb2 67.11(10) 7_666 . ?
Sb1 S4 Sb2 138.33(6) 3_556 . ?
Sb1 S4 Sb2 138.33(6) 3 . ?
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Fe S4 Sb2 126.9(2) 5_666 . ?
Sb1 S4 Sb2 77.29(8) 7_667 . ?
Sb1 S4 Sb2 77.29(8) 7_665 . ?
Fe S4 Fe 117.5(3) . 3_556 ?
Fe S4 Fe 88.0(2) 1_556 3_556 ?
Sb1 S4 Fe 146.5(2) 7_666 3_556 ?
Sb1 S4 Fe 44.03(15) 3_556 3_556 ?
Sb1 S4 Fe 74.41(14) 3 3_556 ?
Sb2 S4 Fe 42.32(9) 3_556 3_556 ?
Fe S4 Fe 92.54(6) 5_666 3_556 ?
Sb1 S4 Fe 100.99(5) 7_667 3_556 ?
Sb1 S4 Fe 138.84(6) 7_665 3_556 ?
Sb2 S4 Fe 136.4(2) . 3_556 ?
Fe S4 Fe 88.0(2) . 3 ?
Fe S4 Fe 117.5(3) 1_556 3 ?
Sb1 S4 Fe 146.5(2) 7_666 3 ?
Sb1 S4 Fe 74.41(14) 3_556 3 ?
Sb1 S4 Fe 44.03(15) 3 3 ?
Sb2 S4 Fe 42.32(9) 3_556 3 ?
Fe S4 Fe 92.54(6) 5_666 3 ?
Sb1 S4 Fe 138.84(6) 7_667 3 ?
Sb1 S4 Fe 100.99(5) 7_665 3 ?
Sb2 S4 Fe 136.4(2) . 3 ?
Fe S4 Fe 39.87(6) 3_556 3 ?

_diffrn_measured_fraction_theta_max    0.371
_diffrn_reflns_theta_full              29.70
_diffrn_measured_fraction_theta_full   0.371
_refine_diff_density_max    0.959
_refine_diff_density_min   -1.300
_refine_diff_density_rms    0.291
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