

long des axes ternaires hélicoïdaux en mettant en commun une de leurs arêtes. Les files d'octaèdres ainsi constituées sont, d'autre part, liées les unes aux autres par les groupements sulfites. La disposition est telle que les atomes de soufre se trouvent à une distance minimale de 3,602 (3) Å, leur centre étant situé sur des cylindres de 4,16 Å de diamètre dont les axes coïncident avec les axes $\bar{3}$ du réseau (Fig. 3). L'absence d'atome à l'intérieur de ces cylindres, laisse apparaître des canaux parallèles à la direction [00.1]. Ceux-ci doivent être en partie occupés par la paire libre du soufre et le nuage électronique de l'atome d'oxygène O(3).

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HgBi₂S₄: Crystal Structure and Relationship with the Pavonite Homologous Series

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Abstract

HgBi₂S₄ is monoclinic, *C*2/*m*, with *a* = 14.17 (1), *b* = 4.06 (1), *c* = 13.99 (1) Å, β = 118.27 (1)°, *Z* = 4. Its crystal structure (*R* = 0.10) contains two (Hg/2), two Bi and four S atoms in the asymmetric unit. $\frac{1}{2}$ Hg(1) and $\frac{1}{2}$ Hg(2) are coordinated by S atoms in flattened octahedra. Bi(1) has a square-pyramidal coordination which approaches sixfold octahedral. Bi(2) is seven-coordinated in a distorted trigonal-prismatic coordination with an extra bond through one face. HgBi₂S₄ has a two-layer structure similar to the member ³*P* (~CuBi₅S₈) of the pavonite homologous series. It differs in a relative displacement of one layer against the other by *b*/2 compared with ideal ³*P*.

Introduction

HgBi₂S₄ was prepared by Brower, Parker & Roth (1973) during studies of non-oxide materials which could be used as optical modulators. The related

system Hg–Sb–S was also investigated by the same workers for similarly suitable compounds. They found that the mineral livingstonite, HgSb₄S₈ (Niizeki & Buerger, 1957; Srikrishnan & Nowacki, 1975), could not be synthesized, nor could the related HgS:2Sb₂S₃ (HgSb₄S₇) on the binary join.

The crystal structures of synthetic silver and copper bismuth sulphosalts have been discussed by Makovicky, Mumme & Watts (1977). The pavonite homologous series *M*_{*N*+1}Bi₂S_{*N*+5} was defined, with the members of the series, in order of increasing *N* (2, 3, 4, 5 and 7), ~PbBi₄S₇ (Takeuchi, Takagi & Yamanaka, 1974), ~CuBi₅S₈ (or Cu_{1.6}Bi_{4.8}S₈) (Ohmasa & Nowacki, 1973), Cu_{2+x}Bi_{6-x}S₉ (*x* = 1.21) (Ohmasa, 1973), Ag₂Bi₆S₁₀ (pavonite), and ~Ag₃Bi₇S₁₂ (benjaminite) (Makovicky & Mumme, 1979). Members of this series are denoted by ^{*N*}*P*. They represent sulpho-salt structures with thinner slabs of octahedra and paired square pyramids, alternating with galena-like slabs of variable thickness (*N*).

In the same study, the relationship between the structures of livingstonite and members of the pavonite

series was discussed. Although similarities were seen to exist, it was concluded that pure Sb structures of the pavonite type may not form because Sb does not easily adopt a regular coordination octahedron. However, the crystal parameters reported for HgBi_2S_4 by Brower *et al.* (1973), and its chemistry, suggested to us that this compound was a member of the pavonite series, probably *ideal* 3P . This was significant because the 3P homologue already established for the series ($\sim\text{CuBi}_5\text{S}_8$ or $\text{Cu}_{1.6}\text{Bi}_{4.8}\text{S}_8$) differs slightly in its crystal structure and chemistry from the ideal member 3P (M_6S_8). In $\text{Cu}_{1.6}\text{Bi}_{4.8}\text{S}_8$, Cu occupies the single coordination octahedron of the thin slabs as two statistical half-atoms in flattened tetrahedra. The crystal structure of HgBi_2S_4 was therefore studied in detail.

Experimental

HgBi_2S_4 was prepared by solid-state reaction of HgS and Bi_2S_3 in 1:1 stoichiometric proportions in a sealed silica tube at 923 K. The powder diffractometer pattern from the compound thus formed corresponded to that previously reported (Brower *et al.*, 1973). Cell dimensions, obtained from Weissenberg films, were also close to those reported previously, and the space-group alternatives agreed. The powder data (Table 1) were collected on a Philips diffractometer, from specimens internally calibrated with KCl ($a = 6.2929 \text{ \AA}$) with Cu $K\alpha$ radiation. They were refined by least squares to give the lattice dimensions shown in Table 2. Intensities $h0l$, $h1l$ and $h2l$ were collected with an integrating Weissenberg camera, multiple-film packs and Cu $K\alpha$ radiation. Corrections for Lorentz, polarization and absorption effects were applied. Visual measurement of intensities was necessary because of the relatively poor quality of the crystals, which made diffractometry an unsatisfactory procedure (Mullen, 1974). Reasonably good

Table 1. *X-ray powder data for HgBi_2S_4 (Cu $K\alpha$ radiation; KCl internal standard with $a_0 = 6.2929 \text{ \AA}$)*

$h k l$	$\sin^2 \theta$ (obs.) ($\times 10^3$)	$\sin^2 \theta$ (calc.) ($\times 10^3$)	$h k l$	$\sin^2 \theta$ (obs.) ($\times 10^3$)	$\sin^2 \theta$ (calc.) ($\times 10^3$)
0 0 2	1567	1567	5 1 0	13154	13151
2 0 1	2645	2650	0 0 6	14106	14100
2 0 3	2853	2854	0 2 0	14313	14464
1 1 0	4019	3995	6 0 6	14645	14653
2 0 2	4564	4557	2 0 5	14979	14979
4 0 2	4770	4742	1 1 5	15633	15618
1 1 $\bar{1}$		4753	2 2 $\bar{1}$		15639
2 0 4	4860	4864	1 1 $\bar{6}$	15951	15898
4 0 0	6105	6104	5 1 $\bar{6}$	16272	16267
0 0 4	6290	6270	5 1 2	18365	18380
3 1 $\bar{2}$	6414	6417	3 1 $\bar{7}$	18534	18550
3 1 0	7057	7047	2 2 $\bar{4}$	19313	19317
3 1 $\bar{3}$	7295	7277	4 0 $\bar{8}$	19438	19454
3 1 1	8534	8537	1 1 $\bar{7}$	20632	20634
2 0 4	10734	10722	0 2 4	20738	20721
5 1 $\bar{2}$	11088	11056	3 1 $\bar{8}$	23319	23326
2 0 6	11253	11232	0 0 8	25061	25067
1 1 4	11726	11726	2 2 4	25197	25176
1 1 $\bar{5}$	11952	11956	6 0 $\bar{9}$	25683	25687
6 0 $\bar{5}$	12564	12541	2 0 7	25836	25844

Table 2. *Crystallographic data for HgBi_2S_4*

Space group	$C2/m$
a	14.17 (1) \AA
b	4.06 (1)
c	13.99 (1)
β	118.27 (1) $^\circ$
D_c	7.00 Mg m^{-3}
Z	4
Radiation	Cu $K\alpha$
Total number of reflections	350
μ	145.3 mm^{-1}

agreement between equivalent reflections on the Weissenberg films was observed. The discrepancy between sixty equivalent reflections, twenty from each level, was 5.8% after absorption corrections for a thin plate were applied.

Structure determination and refinement

The lattice parameters of the 3P homologue, $\sim\text{CuBi}_5\text{S}_8$, are $a = 13.21$, $b = 4.02$, $c = 14.17 \text{ \AA}$, $\beta = 115.6^\circ$, while those of HgBi_2S_4 are $a = 14.17$, $b = 4.06$, $c = 13.99 \text{ \AA}$, $\beta = 118.3^\circ$ (both structures belong to the same space group, $C2/m$). The atomic coordinates of the $\sim\text{CuBi}_5\text{S}_8$ structure (Ohmasa & Nowacki, 1973) were used as a starting point for HgBi_2S_4 , with the Hg atoms in octahedral coordination at point positions (a) 000 and (d) $0\frac{1}{2}\frac{1}{2}$.

With only the $h0l$ data, good agreement between observed and calculated structure factors was achieved with the ideal 3P model projected on to (010). However, bond-length calculations with the refined atomic parameters resulted in two short interactions [Bi(2)–S(4) = 2.6, Bi(2)–S(1) = 2.5 \AA] anomalously distributed along a diagonal within the proposed Bi(2) S_6 octahedron, when the atomic levels in 3P were used. Subsequent three-dimensional structure factor calculations showed that while the 3P positions projected on to (010) are approximately correct for HgBi_2S_4 , the levels of Bi(1), Hg(2), S(3) and S(4) are shifted by $b/2$. With this slightly modified 3P arrangement, the three-dimensional data were refined, with anisotropic

Table 3. *Atomic parameters ($\times 10^4$) with e.s.d.'s in parentheses*

Equipoint	x	y	z	$B (\text{\AA}^2)$
Hg(1)	a	0	0	2.3 (2)
Hg(2)	c	0	0	2.4 (2)
Bi(1)	i	2260 (5)	0	3679 (4)
Bi(2)	i	3499 (5)	0	1379 (5)
S(1)	i	1859 (27)	$\frac{1}{2}$	648 (28)
S(2)	i	4991 (23)	$\frac{1}{2}$	1701 (27)
S(3)	i	1244 (26)	$\frac{1}{2}$	4280 (25)
S(4)	i	3432 (30)	$\frac{1}{2}$	3243 (35)

Table 4. *Interatomic distances (Å) and bond angles (°)*

Hg(1)—S(2)	2.39 (4) × 2	S(2)—Hg(1)—S(1)	96.5*
S(1)	3.10 (4) × 4	S(2)—Hg(1)—S(1)'	83.5
		S(1)—Hg(1)—S(1)''	98.2
		S(1)—Hg(1)—S(1)'''	81.8
Hg(2)—S(4)	2.41 (4) × 2	S(4)—Hg(2)—S(3)	93.4
S(3)	3.15 (4) × 4	S(3)—Hg(2)—S(3)'	80.2
		S(3)—Hg(2)—S(3)''	99.8
		S(4)—Hg(2)—S(3)'''	86.6
Bi(1)—S(3)	2.63 (3) × 1	S(3)—Bi(1)—S(3)'	86.5
S(3)'	2.84 (4) × 2	S(3)—Bi(1)—S(4)	88.9
S(4)	2.87 (3) × 2	S(3)—Bi(1)—S(3)''	91.4
S(2)	3.09 (4) × 2	S(4)—Bi(1)—S(4)	90.2
Bi(2)—S(1)	2.63 (3) × 1	S(3)—Bi(1)—S(4)	89.0
S(2)	2.81 (4) × 2	S(1)—Bi(2)—S(1)'	84.6
S(1)'	2.88 (4) × 2	S(1)—Bi(2)—S(2)	85.4
S(4)	3.34 (4) × 2	S(1)—Bi(2)—S(1)	89.4
		S(2)—Bi(2)—S(2)'	92.6
		S(1)—Bi(2)—S(2)	88.1
		S(1)—Bi(2)—S(4)	62.2
		S(2)—Bi(2)—S(4)	74.5
		S(4)—Bi(2)—S(4)'	74.8

* The e.s.d. for bond angles is 0.6°.

temperature factors for all atoms, to $R = 0.10$.* Neutral-atom scattering curves were used (Cromer & Waber, 1965) and anomalous-dispersion corrections were made for Hg and Bi. Refinement was by a local version of *ORFLS* (Busing, Martin & Levy, 1962) with application of the weighting scheme of Cruickshank, Pilling, Bujosa, Lovell & Truter (1961). Final positional parameters are in Table 3, interatomic distances and bond angles in Table 4.

Description of the structure

HgBi₂S₄ contains two independent Bi atoms, two independent Hg/2 atoms and four independent S atoms. Bi(1) is coordinated by six S atoms (five close and one more distant) at 2.62 (×1), 2.83 (×2), 2.87 (×2) and 3.09 (×1) Å. Its coordination is fivefold square pyramidal, approaching (distorted) octahedral. Bi(2) is bonded to five near and two more distant S atoms at 2.60 (×1), 2.82 (×2), 2.88 (×2) and 3.34 (×2) Å, in a distorted trigonal-prismatic coordination, capped on one face. Hg(1) and Hg(2) are both octahedral. Each has two S atoms much closer than the other four, and linked to the Hg atoms by linear

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35126 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

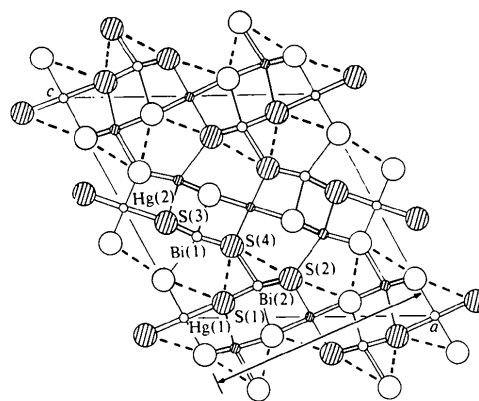


Fig. 1. Crystal structure of HgBi₂S₄ projected on to (010). Smaller circles, Hg and Bi (as labelled); large circles, S. Open circles are at $y = 0$, hatched circles at $y = \frac{1}{2}$. The edge-sharing group of three members which is discussed in the text is marked.

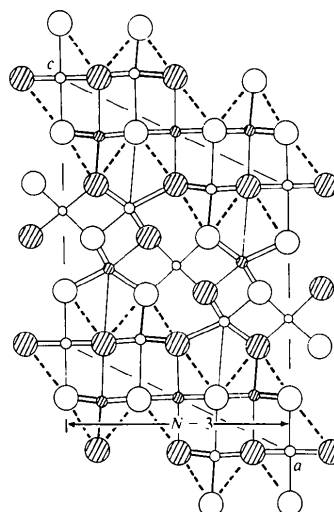


Fig. 2. Crystal structure of $\sim\text{CuBi}_5\text{S}_8$ projected on to (010). Small circles, Cu; medium circles, Bi; large circles, S. Relative levels are as indicated in Fig. 1. $\sim\text{CuBi}_5\text{S}_8$ is the 3P homologue of the pavonite series. The chain of $N = 3$ edge-sharing octahedra is marked.

diagonal bonds. For Hg(1), bonds are 2.39 (×2) and 3.10 (×4) Å; for Hg(2) 2.41 (×2) and 3.15 (×4) Å.

The overall structure (Fig. 1) consists of two layers. One layer contains flattened Hg(2)S₆ octahedra with paired square pyramids of Bi(1), very similar to the thinner slab found in members of the pavonite series (Makovicky *et al.*, 1977). The second layer is composed of the flattened Hg(2) octahedra and pairs of Bi(2) atoms in capped trigonal-prismatic coordinations. Compared with ideal 3P (Fig. 2), one layer in HgBi₂S₄ is displaced by $b/2$ against the other. The same displacement occurs in livingstonite, where matching layers are also shifted by $b/2$ in comparison with pavonite-series homologues (Makovicky *et al.*, 1977).

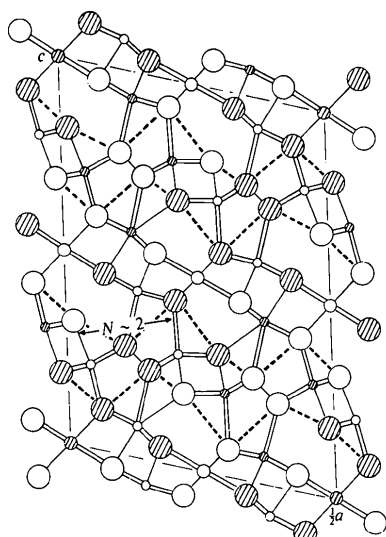


Fig. 3. Crystal structure of livingstonite projected on to (010). Small circles, Sb; medium circles, Hg; large circles, S. Relative levels are as indicated in Fig. 1. Livingstonite approximates to pavonite homologue 2P . The chain of width $N \sim 2$ is marked.

In livingstonite (Fig. 3) the $[\text{Sb}_2\text{S}_4]$ slab only approximates to $N = 2$ with S_2 groups compensating for the relatively small dimensions of the $[\text{SbS}_5]$ pyramids in that structure, compared with larger $[\text{BiS}_6]$ octahedra which occur in pavonite-series homologues. HgBi_2S_4 more closely approximates to 3P because of the ability of the Bi trigonal prisms to edge-share with the Hg(1) octahedra, forming a group or chain three members long.

Discussion

Because of the constraining nature of the short linear bonds in the $\text{S}(2)\text{—Hg}(1)\text{—S}(2)$ group in HgBi_2S_4 , the p^3 bonding of Bi(2) inverts its orientation with respect to that of the matching atoms in the pavonite-series member 3P ($\sim\text{CuBi}_2\text{S}_8$). A comparison of Figs. 1 and 2 shows that, in HgBi_2S_4 , the shortest bonding interaction becomes Bi(2)—S(2) rather than Bi(2)—S(4). The layer shift of $b/2$ is necessary to avoid the second close and unfavourable interaction between Bi(2) and S(4), and the slab is no longer composed entirely of edge-shared octahedra, which is the characteristic of pavonite homologues. $\sim\text{CuBi}_2\text{S}_8$ remains the 3P -type homologue of the pavonite series, and HgBi_2S_4 is not a true member.

However, a series of Hg—Bi compounds, with structures more closely related to pavonite, may exist in which a thinner layer of composition $[\text{HgBi}_2\text{S}_4]$ contains HgS_6 octahedra and paired square pyramids of Bi similar to HgBi_2S_4 . Thicker *octahedral* layers of the type observed in pavonite and benjaminite, with

Table 5. Hg—S bond distances (Å) in sulphosalts

Mineral	Bond distances	Coordination	Reference
(1) Livingstonite	2.52–3.34 1.90–3.41	[2 + 4] linear to [2 + 4] octahedral	(a)
(2) Vrbaité	2.57–2.58 2.37–2.40 (or 2.37–2.86)	[4] tetrahedral [2] linear or with [3] extra long bond	(b)
(3) Galchaite	2.50	[4] tetrahedral	(c)
(4) Christite	2.46–2.66	[4] tetrahedral	(d)
(5) Schwarzite	2.34	[4] tetrahedral	(e)
(6) HgBi_2S_4	2.39–3.10 2.41–3.15	[2 + 4] linear to [2 + 4] octahedral	(f)

References: (a) Srikrishnan & Nowacki (1975). (b) Ohmasa & Nowacki (1971). (c) Divjaković & Nowacki (1975). (d) Edenharter (1976). (e) Kalbskopf (1971). (f) This study.

composition $[\text{M}_N^{\text{oct}}\text{S}_{N+1}]$ could include Ag to maintain balanced valence charges, *i.e.* $[\text{Ag}_{N/2-1}\text{Bi}_{N/2+1}\text{S}_{N+1}]$. The composition of members of this series would be described by the general formula $\text{HgAg}_{N/2-1}\text{Bi}_{N/2+1}\text{S}_{N+2}$ ($N > 2$). Such a structural arrangement requires some Ag, Bi disorder in the thicker slabs, but as this has already been established in benjaminite ($\sim\text{Ag}_3\text{Bi}_7\text{S}_{12}$, 7P) (Makovicky & Mumme, 1979; Herbert & Mumme, 1980), it may not be the limiting factor for structure formation.

Hg—S distances and coordinations in sulphosalts structures have been summarized by Edenharter (1976). Livingstonite, HgSb_4S_8 , vrbaité, $\text{Hg}_3\text{Ti}_4\text{As}_8\text{Sb}_2\text{S}_{20}$ (Ohmasa & Nowacki, 1971), galchaite, $[\text{Hg}_{0.76}\text{(Cu,Zn)}_{0.24}]_{12}\text{Ti}_{0.96}(\text{AsS}_3)_8$ (Divjaković & Nowacki, 1976), and christite, HgTiAsS_3 , were discussed. Schwarzite (mercurean tetrahedrite), in which Hg substitutes for the tetrahedrally coordinated Cu atoms (Kalbskopf, 1971), and HgBi_2S_4 , with linear (to octahedral) coordinations, are also examples of the two coordinations which Hg typically adopts in sulphosalts (Table 5), *i.e.* twofold linear and tetrahedral. These coordinations are also found in the dimorphs of HgS. In cinnabar (Aurivillius, 1950; Auvray & Genet, 1973), the low-temperature form, Hg—S distances in the spiral chains which form the basis of the structure are 2.37 Å with S—Hg—S almost linear (172.8°). Metacinnabarite (Aurivillius, 1964) has the sphalerite structure with Hg tetrahedrally bonded to four S atoms at equal distances of 2.54 Å.

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The Structure of Mooreite

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Abstract

Mooreite, Mg_{9.10}Zn_{4.04}Mn_{1.89}(SO₄)₂(OH)₂₆·8H₂O, from Sterling Hill, New Jersey, crystallizes in space group *P*2₁/*a* with *a* = 11·147 (3), *b* = 20·350 (6), *c* = 8·202 (3) Å, β = 92·69 (4)°, and *Z* = 2. The crystal structure has been determined by Patterson and Fourier methods from 3276 graphite-monochromatized Mo *K*α data and refined by least-squares methods (including the H atoms) to an *R* value of 0·066 (*R*_w = 0·028). The fundamental building units of the structure are brucite-like sheets of edge-sharing Mg octahedra, with ideal composition [Mg_{4.5}(OH)₁₁]²⁻, oriented parallel to (010) and separated by ½*b*. The vacant octahedral sites in these sheets share their upper and lower faces with tetrahedral [Zn(OH)₄]²⁻ groups, each projecting a vertex into the interlayer region. Tetrahedron vertices from opposite sides of adjacent sheets are in turn shared (in a *cis* relationship) with otherwise insular Mn(OH)₂(H₂O)₄ octahedra sandwiched between the sheets. Aside from several rather weak hydrogen bonds between the hydroxyl groups and water molecules, the corner-sharing between Zn tetrahedra and Mn octahedra is the only connection between the brucite layers, thereby accounting for the perfect {010} cleavage and platy habit of the mineral. The sulphate groups occupy large cavities between the Mn octahedra in the interlayer region and are held rather loosely in

position by hydrogen bonding alone. Up to 12% of the cations are disordered over the octahedral sites in both the brucite and Mn layers, but this has no significant effect on the polyhedron bond lengths.

Introduction

The rare mineral mooreite, previously (Mg,Zn,Mn)₈-(SO₄)(OH)₁₄·3–4H₂O with *Z* = 4, occurs as transparent, tabular crystals in cavities and veinlets in massive calcite–franklinite–willemite ore at Sterling Hill, New Jersey (Bauer & Berman, 1929). Subsequent studies by Prewitt-Hopkins (1949) and Finney (1969) concentrated on chemical and physical properties of the mineral, but disagree on the unit-cell dimensions and symmetry, and also on the number of water molecules in the structural formula. Using a new set of chemical data and preliminary results from the present crystal structure analysis Hill (1979) determined that there are only 7·5 cations in the asymmetric unit and proposed the new formula Mg_{9.10}Zn_{4.04}Mn_{1.89}(SO₄)₂(OH)₂₆·8H₂O with *Z* = 2. Information was also provided on the unit-cell dimensions and space-group symmetry (included in the *Abstract*), along with the X-ray diffraction pattern and infrared absorption spectrum. The detailed results of the crystal structure analysis are presented herein. Material for the in-