American Mineralogist, Volume 63, pages 1153–1161, 1978

Polhemusite, a new Hg–Zn sulfide from Idaho

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Abstract

Polhemusite, empirically $Hg_{0.15}Zn_{0.87}Fe_{0.01}S_{0.97}$, is a microscopic constituent of mercury-bearing antimony ore from the B and B deposit, Big Creek district, Valley County, Idaho. Polhemusite occurs as stubby tetragonal prisms, dipyramids, and irregular grains associated with stibnite, cinnabar, mercurian sphalerite, and zincian metacinnabar in a quartz lode. Polhemusite is black, resinous to adamantine, locally with dark red internal reflection.

X-ray diffraction data for polhemusite can be indexed according to a primitive tetragonal cell having $a = 8.71$, $c = 14.74$A. A pseudocubic subcell, $a = 5.33$A, is also present. Possible space groups are $P4/n$, $P4_2/n$, $P4/nbm$, $P4/nmm$, $P4_2/nnm$, and $P4_2/ncm$. Single-crystal data and density are lacking, owing to the minute size of the particles. The cell content, Z, is probably about 24 to 32. Stronger lines of Debye-Scherrer and Gandolfi photographs are 3.16 ms, 3.08 vs, 1.888 s, 1.608 ms, 1.222 m, 1.086 m, 1.024 m.

Polhemusite is variable in composition. Microprobe analysis gives, in weight percent, Hg 18.0–34.7, Zn 42.6–54.7, Fe 0.3–0.7, S 24.0–28.9, sum 101.3–102.8. The mean of 15 analyses, each on a separate grain, is Hg 25.8 ± 5.5, Zn 49.1 ± 3.8, Fe 0.5 ± 0.1, S 26.7 ± 1.6, sum 102.1 ± 0.7. Compositional variation results from zoning, as well as from grain-to-grain variation. Limiting compositions are equivalent to $Hg_{0.10}Zn_{0.92}S_{0.99}$ and $Hg_{0.22}Zn_{0.83}S_{0.95}$.

In polished section, polhemusite looks gray in air, much darker in oil. Against stibnite, it is lavender gray to bluish gray. Polishing hardness >stibnite. Reflection pleochroism in aggregates: distinct in air, very slightly brownish gray to slightly lavender gray; conspicuous in oil, light brownish gray (almost yellow) to purplish gray, but partly obscured by internal reflection. Where unobscured by internal reflection, anisotropism is distinct in air, strong in oil. Internal reflection, not everywhere detectable in air, is strong—lavender, pink, reddish orange, dark red; in oil it is strong, red-orange, not visible in all grains. Reflectance at 470, 546, 589, and 650 nm is (R_1, R_2; $(R_1 + R_2)/2$, in parentheses) 20.1–24.4 (21.8), 17.1–18.3 (17.6), 16.5–17.7 (16.9), ~17.9 percent. Bireflectance decreases with increasing wavelength and is effectively absent at 650 nm. $HV_{25} = 220$–333, mean 262. Knee-shaped twins resembling those of rutile are common; other simple twins and some lamellar twins are present. Cleavage or parting is rare. Zoning is conspicuous in some areas.

Polhemusite, except for its reflection pleochroism and anisotropism, somewhat resembles sphalerite, but its quantitative ore-microscopic properties, twin habit, and X-ray diffraction data are distinctive. Its composition overlaps that of the associated mercurian sphalerite. Polhemusite is inferred to be a metastable, disordered form of (Zn,Hg)S—a polymorph of mercurian sphalerite.

Introduction

Polhemusite is a noncubic Hg–Zn sulfide. Though it is optically anisotropic, it looks somewhat like sphalerite, and its composition overlaps that of mercurian sphalerite. Polhemusite is a microscopic constituent of mercury-bearing antimony ore from the B and B deposit, Big Creek district, Valley County, Idaho. The deposit, discovered in 1964, was described by Leonard (1965).

The distinctive optical properties of polhemusite led to its tentative assignment as a new species in 1965. This tentative assignment was confirmed in

0003-004X/78/1112-1153$02.00

1966 by Mrs. Mead's microprobe analysis of several grains, all of them too small to be extracted for X-ray powder diffraction analysis. In 1970, Mr. Richard B. Tripp concentrated several grams of stibnite and associated sulfides by digesting the quartz-rich gangue in hydrofluoric acid. He then picked out cinnabar grains containing black specks that were thought to be metacinnabar. The powder photograph of three of the black specks, each about 20 microns in diameter, was not that of metacinnabar; it was, by a lucky accident, a photograph of a pure sample of the only other black mineral in the specimen—very spotty because of the size of the particles, but lacking the strong lines of the other minerals already identified in the specimen. Mr. Tripp then mounted the particles in a Gandolfi camera. The excellent Gandolfi record proved to be both unique and indexable on the basis of a tetragonal cell assumed from the morphology. To confirm the assumed cell, the particles were dissolved off their gelatine sliver for remounting of the largest particle in a precession camera, but the only particle large enough for precession photography was lost in the attempted remounting. No other pure particles of suitable size have been found in searching a large suite of samples. That the three particles originally photographed do indeed correspond to the mineral optically and chemically characterized as polhemusite has been confirmed by X-ray powder photography of several samples of mixtures, all of whose constituents were known.

The mineral is named *polhemusite* for the late Clyde Polhemus Ross, born Clyde Polhemus, a student of mercury deposits and of the geology of Idaho, and a member of the U.S. Geological Survey for more than 40 years. The mineral and the name have been approved by the IMA Commission on New Minerals and Mineral Names.

Setting and mineralogy of the deposit

The B and B deposit is a replacement deposit of stibnite and associated mercury minerals in a quartz lode. The lode is part of a large silicified zone in granodiorite of the Idaho batholith. The silicified zone, accompanied by a swarm of rhyolite and latite dikes of Tertiary age, is now known to occupy one of the systems of ring fractures of the Thunder Mountain caldera, a major collapse structure whose center is 14 miles (23 km) southeast of the deposit. The hypogene mineral assemblage noted below is Tertiary. Locally it has been altered to stibiconite and other supergene minerals, including metastibnite. The deposit has been mined in a small way, and some tons of cobbed stibnite have been sold.

Gangue minerals of the deposit are quartz, barite, muscovite, illite, zircon, and fluorite.

Quartz of several generations makes up more than 95 percent of the gangue. An earlier generation of quartz is chalcedonic; a later generation is moderately to coarsely crystalline and comb-like; some very late quartz is chalcedonic, forming thin veinlets that cut the comb quartz. The varieties and apparent ages are far more complex than this arbitrary division suggests. All the quartz contains microscopic inclusions, both solid and fluid, that give it a dusty appearance in thin section. Some comb quartz forms lenticles in chalcedony, the medial area between the quartz teeth being filled with stibnite. Some quartz crystals within the comb are twinned according to an undetermined inclined-axis law.

Barite makes up 5–10 percent of some specimens, but it cannot be detected microscopically in other samples. Barite crystals—some of them lightly dusted with cinnabar, others coated with stibnite—partly fill small, irregular fissures in quartz. Beyond the ends of some microscopic fissures of this sort, discontinuous replacement veinlets of barite are present in unfractured quartz. Fluid and solid inclusions are visible in some of the larger barite crystals.

Muscovite can occasionally be found in barren quartz as a fist-sized aggregate of coarse flakes, or as a single small flake in a thin section. Muscovite is little more than a trace constituent of the deposit, but this trace constituent can be found as hand specimens.

Illite, in contrast, has been detected only microscopically. It occurs as isolated wisps and as irregular nets and clouds of flakes within and next to large crystals of quartz. In other specimens, illite and chalcedony are the matrix for angular fragments of strained quartz in microbreccia. The total quantity of illite is small, its occurrence is sporadic, its concentration is too slight for X-ray diffraction analysis, and its identification is therefore tentative. In thin section, the illite looks like sericite but has $2V_x$ rather small; spectrographic analyses of samples that contain several percent of this mica show no K and only 0.05 percent Na. The absence of K eliminates muscovite; scarcity of Na, as well as geologic occurrence, eliminates paragonite; a sufficiency of Al, Fe, and subordinate Mg permits the inference of illite; and illite is a common clay mineral in some other quartz lodes of the district.

Zircon is ubiquitous in trace amounts; a few small crystals, commonly but not everywhere within areas containing illite, are visible in every thin section of ore. Optical identification of the zircon is confirmed by spectrographic analyses (Leonard, 1965) that show 20–50 ppm Zr in samples of the ore.

A single particle of colorless fluorite intergrown with brown sphalerite was recovered from the HF-insoluble residue of one sample. The size of the fluorite particle (~1/5 mm) and the presence in it of fluid and solid inclusions indicate that the particle was not formed during acid treatment of the sample. (The CaF_2 that occasionally forms during HF decomposition of mineral samples is extremely fine-grained, according to George J. Neuerburg, oral communication.) The cell edge of the fluorite is 5.51 ± 0.01A; the refractive index is 1.437 ± 0.001.

The ore minerals of the deposit, listed alphabetically, are arsenopyrite, chalcopyrite, cinnabar, copper, metacinnabar, polhemusite, pyrite, sphalerite, stibnite, tetrahedrite, and unidentified bright minerals. A rough estimate of the abundance of ore minerals in representative samples is: >10 percent—stibnite; 0.1–1 percent—cinnabar, pyrite, sphalerite; 0.001–0.01 percent—metacinnabar, polhemusite, tetrahedrite; trace—arsenopyrite, chalcopyrite, copper, and unidentified minerals.

The composition of some of the ore minerals has been investigated in a preliminary way. Cinnabar contains 1.1–2.7 weight percent Zn. Metacinnabar contains 10.0–17.7 weight percent Zn. Some sphalerite is nearly pure, some contains a little Fe, and some contains as much as 20 weight percent Hg. Some tetrahedrite is argentian, some is mercurian, and some contains both Ag and Hg. Analysis of a random grain of the last variety gave, in weight percent, ~2–4 Ag (distributed inhomogeneously) and ~10 Hg.

Stibnite, pyrite, and sphalerite range from very fine to coarse. All other ore minerals are fine-grained or extremely fine-grained. Only stibnite and cinnabar form discrete veinlets. Both minerals, as well as sphalerite, form replacement patches. Pyrite and arsenopyrite, and some stibnite and polhemusite, are euhedral.

An orderly paragenetic sequence cannot be recognized. Except for the sparsest ore minerals and regardless of the vein or replacement habit of some, all the ore minerals occur somewhere as inclusions in all the others, the pair polhemusite–sphalerite doubtfully excepted, owing to the difficulty of telling one mineral from the other under certain circumstances. We interpret the gross fabric as indicative of a dumped assemblage in which virtually all the ore minerals were precipitated together, only stibnite and cinnabar locally continuing to grow in late veinlets and as perched crystals. An alternative interpretation is that all but the sparsest ore minerals represent multiple generations. The number of generations or redistributions required to account for the complex pattern of inclusions seems improbably large; this, as well as the scarcity of overgrowths and consistent sequential replacement relations, leads us to favor the hypothesis of dumping—the rather sudden deposition of a disequilibrium assemblage in which the elements Hg and Zn entered into cinnabar, metacinnabar, polhemusite, and sphalerite in quite variable proportions.

Appearance and polishing qualities of polhemusite

Grains of polhemusite are too small to be recognized without a microscope. In incident light, under a stereoscopic microscope, polhemusite looks black. Its luster is resinous to adamantine. A dark red internal reflection is visible in some grains. Accordingly, polhemusite resembles livingstonite and some of the ruby silver minerals viewed under similar conditions. Polhemusite is difficult to distinguish from grains of stibnite flecked with cinnabar, and it cannot be distinguished from metacinnabar in incident light.

Specimens of the ore are difficult to polish because they contain minute vugs, not readily sealed by the usual impregnating agents, as well as frangible aggregates of cinnabar and stibiconite. Lead-lap polishing with magnesia can seldom be completed without some plucking of these fine-grained brittle aggregates. Slow, low-pressure polishing with alumina on cloth produces the best surfaces and makes the polhemusite conspicuous by heightening its relief against the softer stibnite. Ultimately polhemusite takes an excellent polish.

Polhemusite does not tarnish in the dry climate of Denver, and it scarcely darkens after a year's exposure to the humid atmosphere of Washington, D.C.

Microscopic properties

Qualitative properties

We thought when we first observed polhemusite in polished section that its qualitative properties were distinctive. They are, but only under favorable conditions. Here a favorable condition is the prevailing occurrence of polhemusite within stibnite. Against stibnite, polhemusite is slightly lavender gray to bluish gray. The lavender tint, as opposed to pink or brown, is better seen at low and medium magnification than at high. Against cinnabar and metacinnabar, polhemusite looks less lavender and more bluish. Polhemusite is considerably darker and harder than these three associated minerals. Viewed against stibnite under a comparison microscope, polhemusite resembles realgar in lavender to bluish gray tint, but the red internal reflection of polhemusite is less pervasive and less conspicuous than that of realgar. The carbon coating applied to specimens prepared for microprobe analysis greatly enhances the lavender tint and positive relief of polhemusite, making this mineral readily distinguishable from all its associates except sphalerite. Under a comparison microscope, polhemusite looks very slightly lavender gray or very slightly brownish gray against sphalerite, but the two minerals are difficult to distinguish in brightness and tint. The sphalerite used as an external standard of comparison was a ferroan variety, $R(\text{air}) = 17.1$ percent at 546 nm.

Sphalerite is present with polhemusite in our samples, but we have not found the two minerals intergrown. Avoiding aggregates, we have scrupulously selected for description and analysis as polhemusite only the mineral that was positively distinguishable on the basis of all its observed properties, beginning with crystal habit (see below). Polhemusite does have properties that are thoroughly distinctive, but unless these are sought, the mineral can be mistaken for many another—notably for sphalerite.

The *reflection pleochroism* of polhemusite in aggregates is weak in air, very slightly brownish gray to slightly lavender gray; distinct in oil, light brownish gray (almost yellowish) to purplish gray but partly obscured by internal reflection. Some elongate crystals having a rectangular cross section are, in air, darker and more bluish $\| l$, lighter and more pinkish or brownish $\perp l$. Other elongate crystals show these relations reversed. A single perfectly-developed bipyramid shows R_O slightly pinkish, R_E slightly bluish, $R_O > R_E$. Cross sections of prisms look gray—either slightly brownish or slightly bluish—and where untwinned are probably optically isotropic, but compositional zoning makes the latter observation uncertain. The orientation of the optical effects can be interpreted several ways, two of which deserve consideration: (1) The relations observed on one perfect bipyramid are valid for all crystals of polhemusite; the sign of the bireflectance of the mineral is therefore (−) in white light, and it follows that *c* is not always the direction of elongation of the lathy sections, and that the tint detected in cross-sections of prisms cannot be distinguished with as much certainty as our reporting suggests. (2) The single bipyramid represents a special case and thus tells only part of the story; the general case is that *c* is always the direction of elongation, and the effects observed on prism cross-sections have been distinguished with certainty; accordingly, the sign of the white-light bireflectance changes from (+) to (−) within the compositional range represented by our samples. At present, we do not have material suitable for the kind of measurement that would suggest the better of these two interpretations.

With polarizer and analyzer slightly uncrossed, the *anisotropism* of polhemusite is moderate in air, but commonly obscured by internal reflection and difficult to detect if polhemusite is completely surrounded by stibnite. In oil, anisotropism is strong but largely obscured by internal reflection. *Internal reflection,* not everywhere detectable in air, is locally strong—lavender, pink, reddish orange, dark red; in oil it is strong in red-orange but not visible in some grains.

Polhemusite occurs mostly in stibnite as minute stubby prisms, as trains and aggregates of prisms, as dipyramids, as droplets, as forms resembling weevils, and as an intergrowth resembling myrmekite (Figs. 1, 2). Extremely thin rims of polhemusite on stibnite are present but rare. Small granules of polhemusite are intergrown with cinnabar, metacinnabar, and quartz. The prisms, dipyramids, and irregular individuals of polhemusite are less than 25 microns long. Some of the prisms are combined with dipyramids, others with the basal pinacoid. Knee-shaped twins resembling those of rutile and cassiterite are common. The angle between the poles of the prism "faces" is 37° for some twins and about 54° for others, the first angle perhaps representing only a foreshortened view of the second as the twins are seen in the polished section. Referred to the X-ray cell provisionally adopted for polhemusite, the composition plane of the knee-shaped twins is {605}. Contact twins in which the prisms meet at right angles are seen less often; twinning here is presumably on {*hkl*}. Some trains of prisms, their long axes parallel, are perhaps {*h*0*l*} contact twins. Broad, discontinuous lamellae seen in one prism cross-section may represent twinning on {*h*0*l*}. Cleavage or parting is rare: (1) trace perpendicular to the prism axis—perhaps {001}; (2) two perpendicular traces parallel to the diagonals of the prism cross-section—perhaps either {*h*0*l*} and {0*kl*}, or {*hhl*}, depending on the bounding forms of the prism. The planes of cleavage (2) look inclined to the *c* axis; their relation eliminates {100} and {010}, or {110}, as possible forms.

Zoning is present, both in euhedral crystals of polhemusite and in granules. The vaguely defined, elliptical, generally brighter core is enveloped by a narrow, generally darker rim. Some individuals are slightly mottled, rather than zoned. In red light (656 nm), zoning is conspicuous, and the brighter area (core, generally) shows strong internal reflection. The possibility that the zoning is instead an overgrowth of polhemusite on sphalerite has been considered and rejected because at shorter wavelengths both core and rim are optically anisotropic, the transition from one to the other is gradational, and there is no perceptible difference in polishing hardness between core and rim. Similar evidence distinguishes mottling from intergrowth, but with greater difficulty.

In thin sections cut as mirror images of the polished sections, polhemusite ranges from translucent yellow through dark orange-red to highly absorbing brown. Pleochroism is weak; refringence and birefringence are very high; mottling and zoning are conspicuous. The stubby prismatic habit of the mineral is easily seen in some myrmekite-like intergrowths with the stibnite host, and a few slender prisms of polhemusite are identifiable in the quartz matrix. Absorption is stronger $\parallel l$ in some prisms and weaker in others. Optic sign and orientation of the optical indicatrix are not determinable, owing to the small size of the crystals.

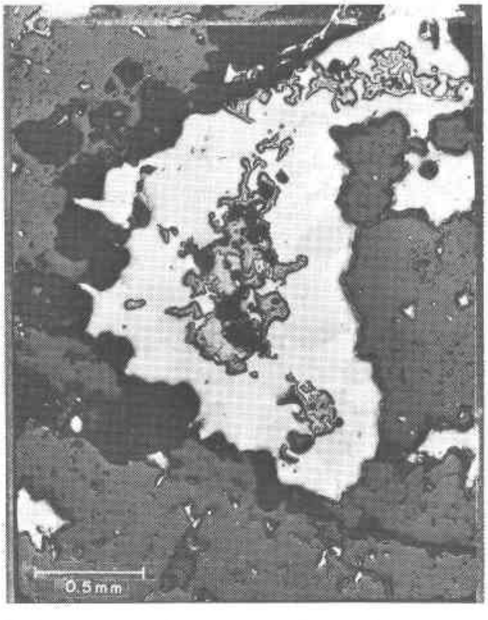

Fig. 1. Aggregates of polhemusite in stibnite. Polhemusite—medium gray, high relief, locally resembling myrmekite. Stibnite—white, distinctly bireflectant. Cinnabar—light gray patches near center. Dark gray matrix—quartz. Black—vugs and pits. Single polar, green filter.

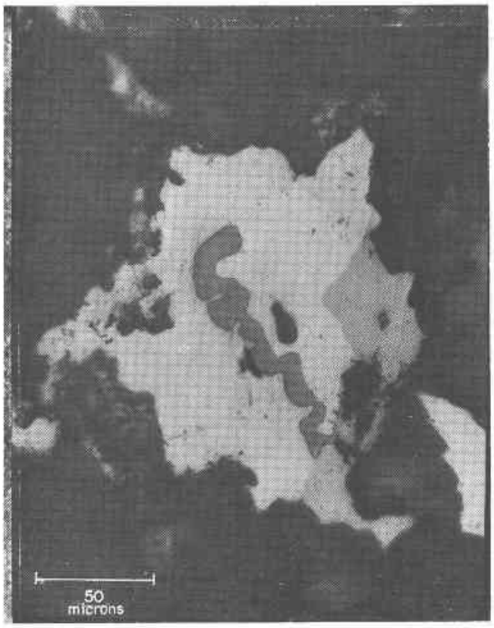

Fig. 2. Train of polhemusite prisms in stibnite. Bluntly terminated knee-shaped twins and linked prisms are faintly mottled. Polhemusite—medium gray. Stibnite—light gray, bireflectant. Medium gray matrix—mostly quartz. Single polar, green filter.

Quantitative properties

Quantitative optical data for polhemusite are given in Table 1. The reflectance and bireflectance at 470 nm look suspiciously high relative to the values measured at longer wavelengths and to the qualitative observations made in white light. Two tests satisfy us that there is no reason to suppose a lower reliability for the blue-light measurements. The slightly ferroan sphalerite (R_{546} = 17.1 percent) previously used with the comparison microscope gave R_{470} = 17.7 percent when measured in series with polhemusite and the carborundum standard. This value is close to the one

Table 1. Reflectance of polhemusite

	R(air),%			
Wavelength, nm	470	546	589	650
R_2	21.3-24.4	17.3-18.3	16.5-17.7	∿17.9
R_1	20.1-22.1	17.1-18.1	16.5-17.5	∿17.9
$R_2 - R_1$ (max. in individual section)	2.3	1.0	0.4	∿0
$(R_1 + R_2)/2$	21.8±1.0	17.6±0.3	16.9±0.5	∿18

Reflectance of three individuals measured by B. F. L. with a Reichert photoelectric microphotometer fitted with a continuous interference filter whose half-width at half-height is 13-15 nm. Carborundum standard N2538.29 calibrated by National Physical Laboratory, Teddington, England. Mount press-leveled on plasticine. The ± value following the mean reflectance is the standard deviation.

obtained by adding the average dispersion of iron-poor sphalerites ($R_{470} - R_{546}$ = 0.6–1.0 percent; see, for example, COM Tables, 1970) to the measured R_{546} of 17.1 percent. The check provided reasonable assurance that the measuring and recording apparatus was not yielding erratic results in the blue. Several areas of polhemusite were then examined visually, from the blue to the red, in light from individual narrow-band interference filters. This examination showed that the bireflectance of polhemusite is rather strong at 482 nm, distinct at 588 nm, and barely distinguishable at 658 nm. The visual observation at 658 nm also confirms the photometric measurements at 650 nm, showing that polhemusite behaves virtually as an isotropic substance at wavelengths near 650–658 nm.

The quantitative color designation of polhemusite is Y = 18.0 percent, x = 0.313, y = 0.304, p_e = 6 percent, $\lambda_d = -536$ nm. The values are derived from the mean reflectance according to the method applied to ore minerals by Piller (1966). Without ambiguity, the brightness value, trichromatic coefficients, excitation purity, and complement of the dominant wavelength state in a formal way what the eye has already seen: that polhemusite is not bright, that it is almost neutral, but that it is definitely purple, the purple character requiring formal expression as the complementary green of wavelength 536 nm.

The microindentation hardness of polhemusite at 25-gram load is 220–333, mean 262, for 13 indentations. The indentations have straight or slightly concave sides and are perfect to slightly fractured. Owing to the small size of the polhemusite individuals, the diameter of the areas indented is about twice the diameter of the indentations—less than ideal but without detectable bias from the matrix of the individuals. The indentations were made with the Vickers diamond pyramid of a Leitz Durimet hardness tester, descent-and-indent period 30 sec, and were measured in nonpolarized green light.

Chemical composition

Electron microprobe analyses (Table 2), made independently by G.A.D. and C.W.M., show that polhemusite varies in composition, as one would expect from the zoning, mottling, and variable reflectance already described. Within the limits of precision of the analyses, the variation in composition is continuous between the observed extremes numbered 1 and 2, Table 2.

The analyses were made on separate grains, each grain representing a polhemusite individual, so far as that could be determined microscopically. Mrs. Mead's analyses were made in 1967 and 1968 by means of a Materials Analysis Company microprobe with an effective take-off angle of 41° at an accelerating voltage of 25 kV. The standards used were ZnS and HgS. LiF crystals were used for the determination of Zn and Hg. A PET crystal was used for the determination of S. The results, corrected for background, drift, and absorption, clearly showed the nature of polhemusite but raised some doubt about the limits of compositional variation. Additional analyses were needed. Mr. Desborough made these in 1972 by means of an ARL-EMX electron microprobe. Three analytical conditions were used with operating conditions, spectral lines, and analyzing crystals as follows: 15 kV, 20 nA specimen current, Hg$M\alpha$–

Table 2. Electron microprobe analyses of polhemusite (weight percent)

	1	2	3	4
Hg	18.0	34.7	25.8±5.5	27.2
Zn	54.7	42.6	49.1±3.8	47.5
Fe	-	-	0.5±0.1*	-
S	28.9	24.0	26.7±1.6	24.6
	101.6	101.3	102.1±0.7	99.3
Atomic Proportions	$(Hg_{0.10}Zn_{0.92})S_{0.99}$	$(Hg_{0.22}Zn_{0.83})S_{0.95}$	$(Hg_{0.15}Zn_{0.87}Fe_{0.01})S_{0.97}$	$(Hg_{0.17}Zn_{0.89})S_{0.94}$

* Range 0.3-0.7, not paired with analyses 1 and 2

1. Grain containing least Hg. L-64-SR7.2, area B. George A. Desborough, analyst.
2. Grain containing most Hg. L-64-SR7.2, area A. George A. Desborough, analyst.
3. Mean, 15 grains. George A. Desborough, analyst.
4. Mean, 6 grains. Cynthia W. Mead, analyst.

ADP, Zn$K\alpha$–LiF, S$K\alpha$–ADP; 15 kV, 20 nA specimen current, Fe$K\alpha$–LiF, Sb$L\alpha$–ADP, S$K\alpha$–ADP; 6 kV, 40 nA specimen current, Hg$M\alpha$–ADP, S$K\alpha$–ADP, S$K\alpha$–ADP, the last two simultaneously on separate spectrometers. The following compounds were used as standards: ZnS, HgS, Ag_2S, HgTe, CdS, PdS, Bi_2S_3, InS, FeS, Sb_2S_3, (Fe,Zn)S. Values for Zn and Fe were obtained from the 15 kV analyses and values for Hg and S from the 6 kV analyses in order to eliminate the need for absorption corrections. The precision of the individual analyses is high: Hg 1.0, Zn 0.5, Fe 0.1, S 0.3, in weight percent.

Minor elements detected in polhemusite are Cu, Fe (Table 2), and Sb. The concentration of Cu and Sb is too low to report in numerical form.

The empirical formulae given in Table 2 are discussed in the section on X-ray data.

The chemical composition of polhemusite overlaps that of mercurian sphalerite and approaches that of zincian metacinnabar.

X-ray diffraction data and notes

X-ray diffraction data for polhemusite, obtained by combining the records from Gandolfi and Debye-Scherrer cameras, are given in Table 3. The data have been indexed according to a primitive tetragonal cell having $a = 8.71$, $c = 14.74$A. Possible space groups are $P4/n$, $P4_2/n$, $P4/nbm$, $P4/nmm$, $P4_2/nnm$, and $P4_2/ncm$. The provisional cell and the space group remain to be confirmed by single-crystal study, but the large value of c is corroborated by a very spotty photograph taken in a Debye-Scherrer camera acting as a crude rotation camera. The photograph shows that the repeat distance along one crystal axis is $\geqq$12A if, as seems likely, the spots are a blurred record of the zero level and first level of a favorably-oriented crystal fragment.

The provisional cell of polhemusite is geometrically plausible in relation to the cells of cinnabar and metacinnabar:

$$a_{\text{plh}} \approx 2a_{\text{cn}} \approx \sqrt{2}a_{\text{mcn}}, c_{\text{plh}} \approx \frac{3}{2}\, c_{\text{cn}}, \; V_{\text{plh}} \approx 8V_{\text{cn}}$$

In relation to the cell of artificial γ-HgS,

$$a_{\text{plh}} = \sqrt{2}a_{\text{r}} \;\text{ of }\; \gamma\text{-HgS}, c_{\text{plh}} \approx c \;\text{ of }\; \gamma\text{-HgS}^{1}$$

Table 3. X-ray data for polhemusite

a = 8.71, c = 14.74Å

h k l	d_{obs}, Å	d_{calc}, Å	I	Camera
110	6.19	6.16	vw	D
111	5.68	5.68	vw	D
112	4.74	4.73	w	D
113	3.83	3.84	w	D
004	3.60	3.68	m	D
212	3.40	3.44	w	D
114	3.13, 3.19	3.16	ms	D, G
220	3.09, 3.08	3.08	s, vs	D, G
301	2.85	2.85	vw	G
115	2.66	2.66	mw	G
304, 314	2.24	2.28, 2.21	w	G
305	2.07	2.07	w	G
403	1.989	1.991	vw	G
333, 422	1.888	1.894, 1.883	s	G
334	1.791	1.793	vw	G
521	1.608	1.608	ms	G
209, 523	1.535	1.535, 1.536	vw	G
614	1.335	1.335	mw	G
615	1.288	1.288	vw	G
4·0·10	1.222	1.221	m	G
642	1.191	1.192	vw	G
801	1.086	1.086	m	G
2·0·14, 558, 661	1.024	1.024	m	G
836? 844?	.9405	.9415, .9414	w	G
765, ...	.8996	.8996	mw	G
775, ...	.8435	.8430	w	G
8·1·12, ...	.8114	.8112	w	G

D—Debye-Scherrer. Film D-8167; reflections very spotty.

G—Gandolfi. Film D-8174; reflections good.

Cameras of diameter 57.3 mm. Cu$K\alpha$ = 1.54178Å, Ni filter; Straumanis film arrangement; film shrinkage negligible. Relative intensities estimated visually—s, strong; v, very; m, medium; w, weak. Gelatine-tip mount of 3 particles.

The unit cell of cinnabar contains 6 atoms—3(HgS)—and the relation $V_{\text{plh}} \approx 8V_{\text{cn}}$ suggests that polhemusite may contain approximately 8 × 6 = 48 atoms. If the total number of atoms is 48, the complete formula of polhemusite becomes $\sim 24(Hg_{0.15}Zn_{0.87}Fe_{0.01}S_{0.97})$. The density of polhemusite could not be measured. We suppose it is greater than that of sphalerite (4.09 for synthetic cubic ZnS) and less than that of metacinnabar (7.71 for synthetic cubic HgS). The calculated density of polhemusite, based on cell volume, empirical composition, and $Z = 24$, is 4.23 g/cm³. This value is plausible but perhaps less than the true density. If $Z = 28$–32 (based on the relation $V_{\text{tetrag.}}/V_{\text{pscub.}} = 7^{+}$), the calculated density of polhemusite becomes 4.93–5.63—also plausible. We conclude, therefore, that Z is probably some number between 24 and 32.

Polhemusite has a pseudocubic subcell with $a = 5.33$A (Drs. D. C. Harris and Akira Kato, 1972, oral and written comments on the IMA abstract proposing the new mineral polhemusite; subcell edge and indexing confirmed by us). Multiples of the subcell

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[1] The cell edges of cinnabar, metacinnabar, and artificial γ-HgS are from Strunz (1970). The data recently reported by Protod'yakonova *et al.* (1971) for natural γ-HgS do not include cell edges.

cannot be conventionally stacked to form a tetragonal cell of the required dimensions. Instead, the fundamental geometric relation is this: two corner-to-corner cubic subcells of polhemusite sit within the tetragonal cell with body diagonals of cubes and parallelopiped coinciding. When the subcells are so positioned, they can be rotated about their body diagonals to bring an appropriate face diagonal d of each subcell close to coincidence with the c direction of the tetragonal cell. The body diagonal of the subcell has a length $l = a\sqrt{3} = 9.23\text{A}$. The body diagonal of the tetragonal cell has a length l of 19.21A. Thus $2l_{\text{pscub.}} \approx l_{\text{tetrag.}}$; $18.46\text{A} \approx 19.21\text{A}$, difference 0.75A. The face diagonal $d_{\text{pscub.}} = a\sqrt{2} = 7.54\text{A}$; $2d_{\text{pscub.}} \approx c_{\text{tetrag.}}$; $15.08\text{A} \approx 14.74\text{A}$. However, the vertical projection of $d_{\text{pscub.}}$ on $c_{\text{tetrag.}}$ is 7.29A, twice it is 14.58A, and the fit parallel to c is good. We emphasize that this is the geometric relation between subcell and tetragonal cell; it is not necessarily the fundamental structural relation.

The existence of the subcell in polhemusite suggested to Dr. Kato (written communication, 1972, 1973) that the fundamental structure of polhemusite is related to the sphalerite structure, though as he pointed out the edge of the subcell of polhemusite is unexpectedly shorter than that of pure ZnS ($a = 5.41\text{A}$). In pure ZnS, the Zn–S distance calculated from atomic coordinates is 2.34A; in pure HgS, isostructural with sphalerite, the Hg–S distance is 2.53A. But in the polhemusite subcell, the interatomic distance is only 2.31A if we assume that the subcell has the sphalerite structure. Therefore, we are disinclined to believe that the polhemusite subcell has the sphalerite structure.

After our manuscript was submitted to the journal, Kato (written communication, 1975) proposed a hexagonal cell for polhemusite, $a = 25.22$, $c = 9.28\text{A}$, cell content $15(\text{Me}_9\text{S}_8)$, Me:S 1.125. The density calculated according to his formula is 4.98 g/cm^3, and his hexagonal cell is related to our tetragonal cell as follows:

$$a_{\text{hex.}} \approx \frac{5}{\sqrt{3}}\, a_{\text{tetrag.}},\; c_{\text{hex.}} \approx \frac{5}{8}\, c_{\text{tetrag.}},\; V_{\text{hex.}} \approx \frac{8}{\sqrt{3}} V_{\text{tetrag.}}$$

Kato's elegant argument for the hexagonal cell and its content is based on the assumption that a sphalerite-like structure of the pseudocubic subcell remains very likely, and on the analogy between polhemusite and nowackiite, hexagonal (rhombohedral) $\text{Cu}_6\text{Zn}_3\text{As}_4\text{S}_{12}$ (Marumo, 1967), which has a sphalerite substructure and Me:S = 1.083. The powder data for polhemusite can be indexed very well according to the proposed hexagonal cell, but the cell must have hexagonal symmetry, not rhombohedral, because some reflections of the type $h\,k\,i\,l$ have $-h + k + l \neq 3$.

Kato's proposed hexagonal cell for polhemusite does not agree with the observed tetragonal morphology. If polhemusite is structurally hexagonal but morphologically tetragonal, the implication is clear: the tetragonal form that we observe in polished sections is a relict form, some tetragonal precursor having inverted to a mineral that is structurally hexagonal. The alternative to inversion is pseudomorphism without preservation of a trace of the original tetragonal host. Until firm structural evidence for a hexagonal cell can be obtained and a tetragonal-to-hexagonal inversion demonstrated experimentally, we are inclined to accept the simpler solution provided by a provisional tetragonal cell that is consistent with the observed morphology.

We speculate that polhemusite may be a disordered high form, metastable in the mineral assemblage of the B and B deposit. Mercurian sphalerite having almost the same composition as polhemusite and associated with it in the B and B assemblage may represent the ordered, low form. The slight metal excess indicated for polhemusite by the microprobe analyses, if real and not due to excessive absorption of S by Zn, might explain the persistence of the disordered form in the assemblage.

Acknowledgments

The following members of the U.S. Geological Survey contributed substantially to this study: Richard B. Tripp undertook the HF decomposition of samples, isolated three polhemusite particles, and mounted the particles for X-ray photography; Keith Robinson listened with patient disbelief to a discussion of the geometric relation of the provisional cell and pseudocubic subcells; he and John W. Adams helpfully reviewed the manuscript; Arthur J. Gude III provided some simple crystal models; Richard B. Taylor, Mrs. William Brennan, and Mrs. Joseph M. Hedricks guided the photographing of polished sections used in microprobe analysis; Mrs. Hedricks made copies of X-ray photos for study by Dr. Kato. Dr. D. C. Harris and Dr. Akira Kato, acting as members of the Commission on New Minerals and Mineral Names, called attention to the pseudocubic cell of polhemusite, and Dr. Kato stimulated much thought on the nature of polhemusite. Professor J. J. Finney, Colorado School of Mines, made the attempt at precession photography of a hopelessly small particle. Dr. Horst Piller, Carl Zeiss/Oberkochen, provided templates that simplified the calculation of color values. William C. Leonard made skeleton models of the tetragonal and cubic cells for his father's use. We are grateful to all these people for their generous help.

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Manuscript received, January 6, 1975; accepted for publication, June 14, 1978.