

Hanawaltite, $\text{Hg}_6^{1+}\text{Hg}_2^{2+}[\text{Cl},(\text{OH})]_2\text{O}_3$ —A new mineral from the Clear Creek claim, San Benito County, California: Description and crystal structure

Andrew C. Roberts

Geological Survey of Canada, 601 Booth Street, Ottawa, Ontario, Canada K1A 0E8

Joel D. Grice and Robert A. Gault

Research Division, Canadian Museum of Nature, Ottawa, Ontario, Canada K1P 6P4

Alan J. Criddle

The Natural History Museum, Cromwell Road, London, England SW7 5BD

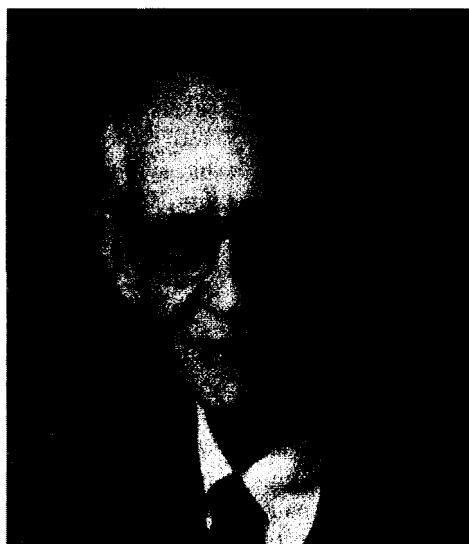
Richard C. Erd

U.S. Geological Survey, 345 Middlefield Road, Menlo Park, California 94025

(Received 9 August 1995; accepted 22 October 1995)

Hanawaltite, ideally $\text{Hg}_6^{1+}\text{Hg}_2^{2+}\text{O}_3\text{Cl}_2$, is orthorhombic, *Pbma* (57), with unit-cell parameters refined from powder data: $a=11.790(3)$, $b=13.881(4)$, $c=6.450(2)$ Å, $V=1055.7(6)$ Å³, $a:b:c=0.8494:1:0.4647$, $Z=4$. The strongest six lines of the X-ray powder-diffraction pattern [d in Å (I)(hkl)] are: 5.25 (80)(111), 3.164 (60)(231), 3.053 (100)(041), 2.954 (70)(141), 2.681 (50)(401), and 2.411 (50)(232,341). The mineral is an extremely rare constituent in a small prospect pit near the long-abandoned Clear Creek mercury mine, New Idria district, San Benito County, California. It was found on a single-fracture surface where it is intimately associated with calomel, native mercury, cinnabar, montroydite, and quartz. Individual crystals are subhedral to anhedral, platy to somewhat bladed, and average about 50 µm in longest dimension. The largest known crystal is approximately 0.3×0.3 mm in size and is striated parallel [001]. Hanawaltite is opaque to translucent (on very thin edges), black to very dark brown—black in color, with a black to dark red—brown streak. Other physical properties include: metallic luster; cleavage {001} good; uneven fracture; brittle; nonfluorescent; $H<5$; calculated density (for the empirical formula) 9.51 g/cm³. In polished section, hanawaltite is moderately to strongly birefractant and is pleochroic white (R_1) to blue—white (R_2). In reflected plane-polarized light, it is white with orange—red internal reflections in very thin grains and at grain margins. The anisotropy is strong with bright metallic blue rotation tints. Measured reflectance values, in air and in oil, are tabulated. Electron-microprobe analysis yielded Hg_2O 82.46, HgO 14.27, Cl 3.33, H_2O [0.34], sum [100.40], less $\text{O}=\text{Cl}$ 0.75, total [99.65] wt. %, corresponding to $\text{Hg}_{6.00}^{1+}\text{Hg}_{1.00}^{2+}[\text{Cl}_{1.43}(\text{OH})_{0.57}]_{\Sigma 2.00}\text{O}_{3.00}$, based on $\text{O}+\text{Cl}=5$. After the crystal structure was determined, the original microprobe value for Hg_2O , 96.2, was partitioned in a ratio of $6\text{Hg}_2\text{O}:\text{HgO}$ and (OH) was calculated, such that $\text{Cl}+(\text{OH})=2$. The hanawaltite structure consists of undulatory $[\text{Hg}-\text{Hg}]^{2+}$ ribbons which roughly parallel (100). The diatomic $[\text{Hg}-\text{Hg}]^{2+}$ groups have anion tails which, in turn, serve as cross linkages between dimer ribbons through $[\text{Hg}_2^{2+}\text{O}_2\text{Cl}_2]$ planar rhombs. The structure is compared to that of other mercury oxychlorides and each is found to have its own unique structural features. This structural diversity is attributed to the inherent ability of mercury to adopt either metallic or ionic types of bonds. The mineral name honors the late Dr. J. D. (Don) Hanawalt (1903–1987), who was a pioneer in the field of X-ray powder diffraction. © 1996 International Centre for Diffraction Data.

Key words: hanawaltite, new mineral species, mercurous mercuric oxychloride, crystal structure, electron-microprobe data, reflectance data, Clear Creek claim, San Benito County, California



J. D. Hanawalt

I. INTRODUCTION

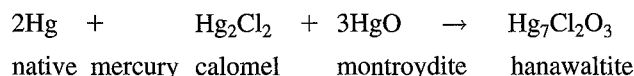
The new mineral species described here, hanawaltite, was first identified by X-ray powder-diffraction analysis in 1991, by one of us (RCE). The rock specimen which was eventually found to contain the mineral had been originally collected in 1962 by amateur mineralogist E. H. Oyler (a specialist in mercury minerals), from a small prospect pit near the long-abandoned Clear Creek mercury mine, New Idria district, San Benito County, California (lat. 36°22'59"N, long. 120°43'58"W). The discovery specimen was part of a float rock which was situated approximately 50 feet west of the discovery boulder containing edoyleite (Erd *et al.*, 1993). The mineral megascopically resembles wattersite (Roberts *et al.* 1991) and thus was not positively identified as a potential new mineral species until subjected to routine X-ray powder-diffraction study. Despite assiduous searches, only one specimen containing crystals of hanawaltite has so far been found.

The mineral is named hanawaltite in honor of the late Dr. J. D. (Don) Hanawalt (1903–1987), a pioneer in the field of X-ray powder diffraction. As noted by Jenkins (1987), "Don Hanawalt is known as the father of the pattern storage and retrieval system still in use today. Indeed, Hanawalt's work in this area while still with the Dow Chemical Company, along with Ludo Frevel and the late Sid Rinn, formed the basis of a qualitative multiphase analysis method which has stood the test of time for more than 50 years." In fact, the search-match method is named in his honor. He was also one of the original founding members of what is currently known as the International Centre for Diffraction Data (ICDD), publisher of the Powder Diffraction File. The mineral and mineral name have been approved by the Commission on New Minerals and Mineral Names, I.M.A. Holotype material, consisting of the type specimen and one polished section, are deposited in the Systematic Reference Series of the National Mineral Collection at the Geological Survey of Canada, Ottawa, Ontario under catalog No. NMC 67396.

II. OCCURRENCE AND ASSOCIATED MINERALS

Hanawaltite is an extremely rare constituent at the Clear Creek claim. Only one hanawaltite-bearing area, a fracture surface measuring 8×2 mm, on a single specimen has been identified to date. On this quartz-rich fracture surface, the mineral occurs as isolated crystals which are intimately associated with greenish-brown resinous calomel, globules of native mercury, red cinnabar, and varicolored (dark red-brown to brown-black to black) montroydite. The host rock is a brecciated silica-carbonate rock which is composed principally of ferroan magnesite and quartz. Other mercury-bearing minerals identified by X-ray powder-diffraction analyses from the Clear Creek claim include edgarbaileyite (Roberts *et al.*, 1990a; Angel *et al.*, 1990), szymańskiite (Roberts *et al.*, 1990b; Szymański and Roberts, 1990), wattersite (Roberts *et al.*, 1991; Groat *et al.*, 1995), deanessmithite (Roberts *et al.*, 1993), edoyleite (Erd *et al.*, 1993), peterbaylissite (Roberts *et al.*, 1995), eglestonite, terlinguaite, schuetteite, mosesite, gianellaite, metacinnabar, and six unnamed mercury-bearing phases that are currently under investigation. A description of the geology of the Clear Creek mercury mine is given by Eckel and Myers (1946); other

references dealing with the geology, geochemistry, and mineralogy of the area surrounding Clear Creek can be found in the paper dealing with edoyleite (Erd *et al.*, 1993). Hanawaltite most probably formed as an alteration product of pre-existing mercury-bearing minerals; one could envisage as a possible reaction:



All four minerals are, indeed, found on the same fracture surface. The scarcity of this new mineral would seem to indicate that primary native mercury, calomel, and montroydite must coexist in intimate association in order for secondary hanawaltite to form.

III. PHYSICAL PROPERTIES

The largest known crystal of hanawaltite, which was subsequently used for single-crystal precession study, crystal-structure analysis, electron-microprobe analysis, and the reflectance study, initially measured approximately 0.3×0.3 mm in size and was somewhat platy in habit. It was subhedral and striated parallel [001] with no observable crystal forms. Other crystals on the specimen are much smaller, tend to be anhedral, and generally do not exceed 50 μm in size; these crystals are somewhat bladed in appearance.

The color varies from black to very dark brown-black. The streak is black to dark red-brown. The mineral is opaque to translucent (on very thin edges), possesses a metallic luster, is brittle, and has an uneven fracture. It is non-fluorescent under both long- and short-wave ultraviolet light and has a good cleavage {001}. The hardness is less than 5 (the mineral does not scratch glass), but a more precise value has not been determined. The density could not be determined due to specimen size limitations and dearth of pure material.

IV. X-RAY SINGLE-CRYSTAL AND POWDER STUDIES

The single, untwinned crystal of hanawaltite, noted earlier, was examined by single-crystal precession methods employing Zr-filtered MoKα radiation. It was initially mounted such that *c** was parallel to the dial axis, then remounted such that *b** was parallel to the dial axis. The following levels were photographed: *h*0*l*→*h*3*l*, 0*kl*→3*kl*, *hk*0→*hk*2, 110*[^]*c** and 102*[^]*b**. Precession films indicate orthorhombic symmetry, and measured unit-cell parameters *a*=11.73, *b*=13.82, and *c*=6.430 Å. There are two systematic absences: *hk*0 with *h*≠2*n* and 0*kl* with *k*≠2*n*; these absences dictate that the permissible space groups are *Pb*2₁*a* (29) or *Pbma* (57) (diffraction aspect *Pb***a*). The correct space group is *Pbma* (57), as determined from crystal-structure studies. The refined unit-cell parameters, *a*=11.790(3), *b*=13.881(4), *c*=6.450(2) Å, *V*=1055.7(6) Å³, and *a*:*b*:*c*=0.8494:1:0.4647, are based on 29 powder reflections representing *d* values between 3.357 and 1.474 Å for which unambiguous indexing was possible, based on both visual inspection of single-crystal precession films and calculated intensities derived from the crystal structure. A fully indexed powder pattern is presented in Table I. The powder data are

TABLE I. X-ray powder data for hanawaltite.

$I_{\text{calc.}}$	$I_{\text{est.}}$	$2\theta_{\text{obs}}$	$d\text{\AA}_{\text{meas}}$	$d\text{\AA}_{\text{calc}}$	hkl	$I_{\text{calc.}}$	$I_{\text{est.}}$	$2\theta_{\text{obs}}$	$d\text{\AA}_{\text{meas}}$	$d\text{\AA}_{\text{calc}}$	hkl
4	10	13.800	6.42	6.45	001	18	20	40.100	2.249	2.247	440
4	5	15.075	5.88	5.90	200	7	20	41.450	2.178	2.178	061
4	5	15.700	5.64	5.66	101	7			2.176		402
4	3	16.275	5.45	5.43	210	8	10	42.225	2.140	2.142	161
46	80	16.900	5.25	5.24	111	10			2.139		351
16	30	18.850	4.71	4.72	021	11	15	42.825	2.112	2.110	521
19	30	19.700	4.51	4.49	220	5	10	44.275	2.046	2.054	023
13				4.39	121	6			2.043		261
21	40	20.425	4.35	4.35	201	13	10	45.400	1.998	1.999	213
10				3.69	221	5	5	46.650	1.947	1.946	610
11	25b	24.300	3.66	3.64	230	4	3	47.100	1.929	1.929	451
11	20	26.550	3.357	3.356	301	10	10	47.775	1.904	1.904	502
3				3.262	311	3	3	48.200	1.888	1.891	620
4	3	27.450	3.249	3.225	002	13			1.867		541
45	60	28.200	3.164	3.170	231	13	30	48.850	1.864	1.863	611
30	20	28.725	3.108	3.111	102	12	10	49.525	1.840	1.843	442
100	100	29.250	3.053	3.056	041	18	30	50.475	1.808	1.809	630
33	20	29.825	2.993	2.991	240	21	40	52.375	1.747	1.746	243
72	70	30.225	2.954	2.958	141	6			1.737		403
30	20	30.625	2.919	2.925	022	9	5	52.775	1.735	1.735	080
24	10	31.025	2.882	2.883	410	20	25	54.400	1.686	1.685	423
20	20	31.625	2.829	2.829	202	4	3	55.825	1.647	1.645	470
16	10	32.250	2.776	2.772	212	4	5	56.575	1.627	1.626	433
16	20	32.925	2.720	2.717	331	5	3	57.075	1.614	1.612	281
49	50	33.425	2.681	2.681	401	8	5	57.625	1.600	1.598	104
27	30	34.750	2.581	2.582	132	17	15	58.250	1.584	1.585	462
12				2.512	250	16	20	58.600	1.575	1.575	063
10	30	35.975	2.496	2.501	421	6	10	59.475	1.554	1.553	443
16				2.493	302	4			1.552		372
20	20	36.625	2.454	2.454	312	11	10	61.150	1.516	1.515	182
30				2.414	232	13	15	62.025	1.496	1.495	480
16	50	37.300	2.411	2.413	341	5			1.474		234
2				2.363	042	7	20	63.050	1.474	1.473	453
6	10	38.275	2.351	2.341	251	4			1.470		562
14				2.320	431	8	10	63.975	1.455	1.454	291
10	20	38.850	2.318	2.314	060						

114.6 mm Debye-Scherrer powder camera; Cu radiation, Ni filter (λ CuK=1.54178).

Intensities estimated visually; b=broad line.

Calculated intensities derived from crystal structure.

Not corrected for shrinkage and no internal standard.

Indexed on $a=11.790$, $b=13.881$, $c=6.450$ Å.

unique and bear no resemblance to any other inorganic phase listed in the Powder Diffraction File. With $Z=4$, the calculated density for the mineral with the empirical formula

$$\text{Hg}_6^{1+}\text{Hg}^{2+}[\text{Cl}_{1.43}(\text{OH})_{0.57}]_2\text{O}_3 \text{ is } 9.51 \text{ g/cm}^3.$$

V. OPTICAL PROPERTIES

A. Qualitative optical properties

As will be expanded upon in the crystal-structure section, hanawaltite decrepitates on exposure to sunlight; therefore, in the microscopic investigation, extra care was taken to check on the response of the mineral to light. Strange to relate, no detectable change was observed in the time required for its description or measurement. In a freshly buffed polished section (MgO in distilled water suspension on Pellon), in plane-polarized light (at 3100 K), hanawaltite varies from a bright bluish white to a somewhat duller, grayish white, i.e., it is bireflectant and slightly pleochroic. Between crossed polars it displays straight extinction—from its one rotation tint, a metallic bluish gray; with the analyzer rotated

from extinction by 3° , the only discernible difference is that the blue color seems more intense. When immersed in oil, these color phenomena are intensified. Internal reflections were not observed in plane-polarized light, neither were they common between crossed polars, though, at some grain boundaries, orange-red reflections were noted, and in one minute fragment of the mineral, the reflections formed a complex pattern reminiscent of opalescence.

B. Reflectance measurements

Measurements were made relative to a Zeiss-calibrated SiC reflectance standard (No. 472) using the Zeiss MPM03 microscope housed at The Natural History Museum, London, England. The largest grain of hanawaltite available for study was approximately $40 \times 20 \mu\text{m}$; this required the use of a $\times 40$ objective (effective NA=0.26) for a measured diameter of $8 \mu\text{m}$.

The reflectance data (Table II) are in accord with the qualitative observations, and are summarized in the table of color values (Table III). These, and Figure 1, the reflectance

TABLE II. Reflectance data for hanawaltite.

λ_{nm}	Reflectance data			
	R_1	R_2	$^{im}R_1$	$^{im}R_2$
400	26.2	37.6	12.2	22.6
420	25.2	34.75	10.9	19.5
440	24.2	32.5	10.1	17.2
460	23.3	30.55	9.43	15.3
470	22.8	29.6	9.17	14.6
480	22.4	28.95	8.92	14.0
500	21.75	27.7	8.45	13.0
520	21.25	26.7	8.15	12.2
540	20.8	25.9	7.85	11.6
546	20.7	25.7	7.79	11.4
560	20.5	25.2	7.63	11.0
580	20.3	24.6	7.48	10.4
589	20.15	24.35	7.42	10.4
600	20.1	24.1	7.43	10.2
620	20.0	23.7	7.40	9.90
640	20.2	23.3	7.46	9.65
650	20.2	23.2	7.48	9.59
660	20.3	23.1	7.54	9.54
680	20.2	22.9	7.51	9.47
700	20.0	22.8	7.39	9.51

spectra in air and oil, show clearly that the mineral is a bright bluish white for the higher reflecting orientation and a more subdued grayish blue at 90° to this; thus, in a quantitative sense, this demonstrates the bireflectance and pleochroism of the mineral. Comparison of the spectral reflectance properties of hanawaltite with other oxychloride minerals of mercury (Figure 2) in QDF3 (Criddle and Stanley, 1993) shows distinct similarities between it and poyarkovite (Vasiliev *et al.*, 1981) and virtual identity for R_1 of hanawaltite and that of terlinguaite. However, the higher reflecting vibration direction of terlinguaite is distinctly different from that of hanawaltite; terlinguaite possesses a reflectance peak (corresponding to an absorption peak) at about 430 nm in the blue region of the visible spectrum.

VI. CHEMISTRY

The largest known crystal of hanawaltite, previously used for both single-crystal precession study and crystal-

TABLE III. Color values for hanawaltite.

	Color values, illuminant C:			
	R_1	R_2	$^{im}R_1$	$^{im}R_2$
x	0.298	0.289	0.290	0.274
y	0.300	0.291	0.289	0.272
$Y\%$	20.7	25.5	7.8	11.3
λ_d	472	474	471	473
$P_e\%$	6.5	10.8	10.9	18.6
	illuminant A:			
	R_1	R_2	$^{im}R_1$	$^{im}R_2$
x	0.437	0.428	0.431	0.413
y	0.401	0.398	0.396	0.390
$Y\%$	20.5	25.0	7.7	10.9
λ_d	483	486	482	486
$P_e\%$	2.8	5.0	4.6	9.1

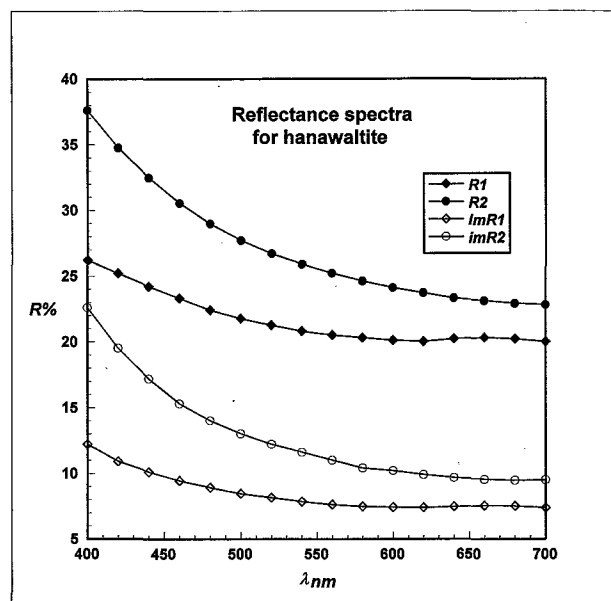


Figure 1. Reflectance spectra measured in air and in oil (N_D 1.515) for hanawaltite. The spectra marked with boxes are those for R_1 and $^{im}R_1$, the + 's are for R_2 and $^{im}R_2$.

structure analysis, was mounted in a polished section and chemically analyzed with a JEOL 733 electron microprobe. The operating conditions were as follows: an operating voltage of 15 kV, a beam current of 20 nA, and a beam 10 μ m in diameter. The sample is approximately 40 $\times$ 20 μ m in size. Natural montroydite (for Hg) and natural mimetite (for Cl) were employed as standards. A 100 s energy-dispersive electron-microprobe scan indicated the absence of all major elements with atomic number greater than 9 other than those reported here; S was specifically sought for, but not found. Only one probe analysis is reported; several analyses were

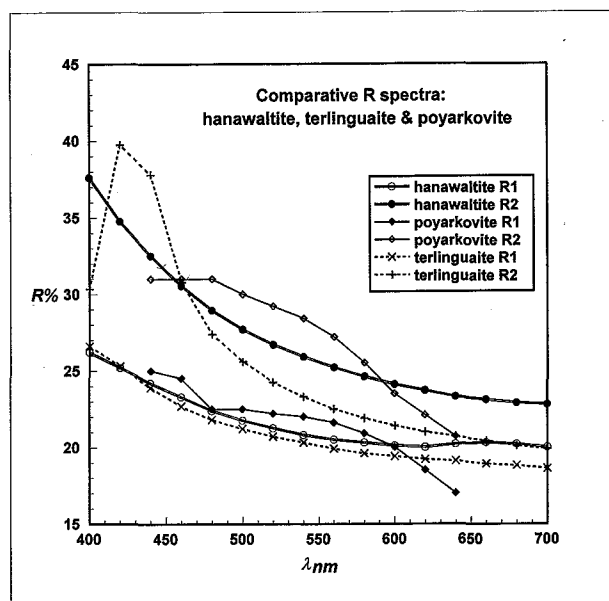


Figure 2. Comparative reflectance spectra for hanawaltite, terlinguaite, and poyarkovite.

TABLE IV. Hanawaltite: data collection summary.

Space group	<i>Pbma</i> (57)	unique reflections	1073
<i>a</i> (Å)	11.777(2)	observed reflections $[F_o > 6\sigma(F_o)]$	751
<i>b</i> (Å)	13.891(3)	μ m (mm ⁻¹ , MoK α)	102
<i>c</i> (Å)	6.460(1)	final <i>R</i> (obs.) %	15.2
<i>V</i> (Å ³)	1056.9(4)	final <i>R</i> _w (obs.) %	13.9
Unit-cell contents 4[Hg ₆ ¹⁺ Hg ₂ ²⁺ Cl ₂ O ₃]		$R_w = [\sum w(F_o - F_c)^2 / \sum w F_o^2]^{1/2}$	$[\sigma^2(F_o)]^{-1}$

attempted, but sample size limitations and decrepitation combined with potential beam overlap with the mounting medium precluded additional reliable results. The analysis gave Hg₂O 96.2, Cl 3.33, sum 99.53, less O=Cl 0.75, total 98.78 wt. %. In light of the crystal-structure determination, the Hg₂O value was recalculated to Hg₂O and HgO in a ratio of 6:1 and (OH) was calculated such that Cl+(OH)=2. This gives Hg₂O 82.46, HgO 14.27, Cl 3.33, H₂O [0.34], sum [100.40], less O=Cl 0.75, total [99.65] wt. %. With O+Cl=5, the empirical formula is Hg_{6.00}Hg_{1.00}²⁺[Cl_{1.43}(OH)_{0.57}]_{Σ2.00}O_{3.00}. The idealized formula is Hg₆¹⁺Hg₂²⁺O₃Cl₂. Other mercury oxychlorides found in nature are: pinchite, Hg₅O₄Cl₂; terlinguaite, Hg₂ClO; comancheite, Hg₁₃(Cl,Br)₈O₉; eglestonite, Hg₆Cl₃O(OH); and poyarkovite, Hg₃OCl.

VII. CRYSTAL-STRUCTURE ANALYSIS

A. Data collection and structure determination

A crystal of hanawaltite, measuring 0.25×0.20×0.08 mm, was used in the crystal-structure data collection on a Nicolet R3m four-circle diffractometer. Intensity data were collected in the manner outlined by Grice (1989). The structure was solved by direct methods which readily located the Hg atomic sites. The structure refined to the *R* values given in Table IV. Reducing the symmetry to the noncentrosymmetric space group *Pb2₁a* (29) did not improve the *R* values. In an attempt to get a better structure refinement a second, larger data collection was carried out. Unfortunately, the second collection, although carried out under the exact same operating conditions, had intensities 40% lower than those of the first experiment. During the year between the two data collections the crystal had been left in a glass vial on open shelving. The material had started to photoreduce to native mercury. Photodecrepitation of hanawaltite was further evidenced by cracks developing in the crystal. This was noted when the crystal was being ground into a plate in order to

reduce absorption effects (Hawthorne *et al.*, 1994). Due to this inherent cracking no further data could be collected on this crystal. Thus the authors were left with only the first data set to work with and thus the critical absorption corrections were meaningless for this size of crystal (i.e., with an absorption coefficient of 102 μm mm⁻¹ there is total absorption for a crystal thickness greater than 0.07 mm; diffraction is from the crystal edges only).

Although the structure refinement is poor, it is all that could be done with the present material. The structure solution is, however, sufficient to determine the chemical formula of the mineral and to delineate the general structural features. The atomic coordinates and isotropic displacement factors are given in Table V and selected bond lengths are given in Table VI.

B. Discussion of the crystal structure

The most significant feature of the hanawaltite structure is the coordination of the two types of Hg ions. There are two, crystallographically distinct pairs of Hg–Hg dimers. These dimers are diagnostic of Hg⁺ ions. The [Hg–Hg]²⁺ pairs form undulatory ribbons approximately parallel (100) (Figure 3). On either end of the Hg1–Hg2 dimer is a pair of O atoms and Cl atoms, whereas on either end of the Hg3–Hg4 pair is a set of differing ligands; with two O atoms and a Cl atom bonded to Hg3, while a single O atom and a single Cl atom are bonded to Hg4 (Table VI and Figure 3). The Hg–Hg bond lengths are typically 2.6 Å and the Hg–O bond lengths are invariably shorter than the Hg–Cl bond lengths. The single Hg²⁺ ion cross links these ribbons by sharing two O atoms and two Cl atoms of adjacent bands in a planar rhomb configuration (Figure 3), giving the structure sets of (001) slabs (Figure 4). The (001) platy habit of the mineral can be attributed to the strong Hg–Hg bonds that lie in this plane (Figure 3) while the good {001} cleavage results from the weak interslab bonding of the [Hg²⁺O₂Cl₂] polyhedron.

TABLE V. Hanawaltite: atomic coordinates and isotropic displacement factors (Å²×10³).

Atomic site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i>
Hg1	0.1167(5)	0.5831(4)	0.4712(8)	1.2(2)
Hg1	0.2911(6)	0.6295(4)	0.6759(9)	1.9(2)
Hg3	0.0378(8)	3/4	0.134(1)	1.6(2)
Hg4	0.2448(9)	1/4	0.151(1)	2.2(2)
Hg5	0	1/2	0	1.0(2)
Cl1	1/4	1/2	0.084(7)	1.4(11)
Cl2	0.44095	3/4	0.329(10)	3.6(15)
O1	0.344(13)	3/4	−0.10(2)	2
O2	−0.020(8)	0.545(7)	0.28(2)	2

TABLE VI. Hanawaltite: selected bond distances (Å).

Hg1–Hg2	2.526(9)	Hg2–Hg1	2.526(9)
Hg1–O2	2.09(10)	Hg2–O1	2.30(10)
Hg1–O2a	2.64(10)	Hg2–O2	2.53(10)
Hg1–Cl1	3.17(3)	Hg2–Cl1	3.23(4)
Hg1–Cl2	3.36(5)	Hg2–Cl2	3.36(5)
⟨Hg1–O⟩	2.365	⟨Hg2–O⟩	2.415
⟨Hg1–Cl⟩	3.265	⟨Hg2–Cl⟩	3.295
Hg3–Hg4	2.56(1)	Hg4–Hg3	2.56(1)
Hg3–O2×2	3.08(10)	Hg4–O1	1.93(15)
Hg3–Cl2	3.20(7)	Hg4–Cl2	2.47(7)
Hg5–O2×2	1.94(10)		
Hg5–Cl1×2	2.994(8)		

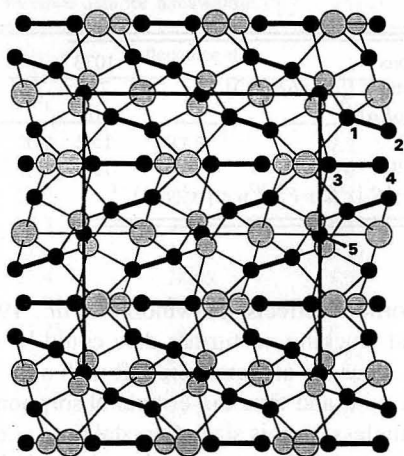


Figure 3. A projection of the structure of hanawaltite on (001) showing Hg atoms as heavily shaded circles and O atoms (small) and Cl atoms (large) as lighter shaded circles. The $[\text{Hg}-\text{Hg}]^{2+}$ dimers with the heavily shaded bonds are in undulating ribbons. The unit cell is outlined with $a < b$ and the integers refer to the Hg atom numbers given in Table V.

Of the other mercury oxychlorides that are known as minerals, three have been subjected to crystal-structure analysis; pinchite (Hawthorne *et al.*, 1994), terlinguaite (Šćavničar, 1956; Brodersen *et al.*, 1989) and eglestonite (Mereiter and Zemmann, 1976; Mereiter *et al.*, 1992). Pinchite does not have any diatomic $[\text{Hg}-\text{Hg}]^{2+}$ groups, whereas the other two minerals have. In eglestonite, the $[\text{Hg}-\text{Hg}]^{2+}$ dimers form columns which are cross linked through shared O atoms; in terlinguaite, O-Hg-O wavy chains are cross linked to Cl-Hg-Hg-Cl "calomel" molecules. Šćavničar (1956) attributes this cross linkage in terlinguaite to a unique triangular configuration of $[\text{Hg}-\text{Hg}]^{2+}-\text{Hg}^{2+}$. In this equilateral triangle the bond lengths are all 2.703 Å (Brodersen *et al.*, 1989).

One might conclude from the uniqueness of each of these structures that mercury oxides and oxychlorides have an inherent ability to attain any one of a variety of chemical combinations through their ability to hybridize the effects of both metallic and ionic bonding. This ability is exemplified in the multitude of varying cation:anion ratios found in these

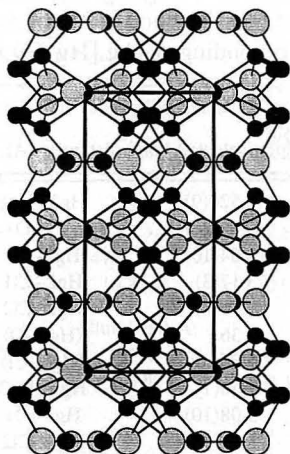


Figure 4. A projection of the structure of hanawaltite on (100) with atom sizes and shading as given in Figure 3. The unit cell is outlined with $c < b$.

compounds. No doubt in the future there will be many more new minerals and synthetics found in this chemical class.

ACKNOWLEDGMENTS

The financial support of a Research Advisory Committee Grant from the Canadian Museum of Nature to JDG is gratefully acknowledged. The authors thank Dr. Frank Hawthorne for the use of the single-crystal diffractometer at the Department of Geological Sciences, University of Manitoba, Mark Cooper, of the same institution, for attempts at thinning the hanawaltite crystal, and Mr. Edward H. Oyler of San Martin, California for the sole hanawaltite-bearing mineral specimen, so generously provided for study.

- Angel, R. J., Cressey, G., and Criddle, A. (1990). "Edgarbaileite, $\text{Hg}_6\text{Si}_2\text{O}_7$: the crystal structure of the first mercury silicate," *Am. Miner.* **75**, 1192–1196.
- Brodersen, K., Göbel, G., and Liehr, G. (1989). "Terlinguaite $\text{Hg}_4\text{O}_2\text{Cl}_2$ —ein mineral mit ungewöhnlichen Hg_3 -baueinheiten," *Z. Anorg. Allg. Chem.* **575**, 145–153.
- Criddle, A. J., and Stanley, C. J. (1993). *The Quantitative Data File for Ore Minerals (Issue 3)* (The Natural History Museum and Chapman and Hall, London), 635 pp.
- Eckel, E. B., and Myers, W. B. (1946). "Quicksilver deposits of the New Idria district, San Benito and Fresno Counties, California," *Calif. J. Mines Geol.* **42**, 81–124.
- Erd, R. C., Roberts, A. C., Bonardi, M., Criddle, A. J., LePage, Y., and Gabe, E. J. (1993). "Edoylerite, $\text{Hg}_3^{2+}\text{Cr}^{6+}\text{O}_4\text{S}_2$, a new mineral from the Clear Creek claim, San Benito County, California," *Mineral. Rec.* **24**, 471–475.
- Grice, J. D. (1989). "The crystal structure of magnolite, $\text{Hg}_2^{1+}\text{Te}^{4+}\text{O}_3$," *Can. Mineral.* **27**, 133–136.
- Groat, L. A., Roberts, A. C., and LePage, Y. (1995). "The crystal structure of watersite, $\text{Hg}_4^{1+}\text{Hg}^{2+}\text{Cr}^{6+}\text{O}_6$," *Can. Mineral.* **33**, 41–46.
- Hawthorne, F. C., Cooper, M., and Sen Gupta, P. K. (1994). "The crystal structure of pinchite, $\text{Hg}_3\text{Cl}_2\text{O}_4$," *Am. Miner.* **79**, 1199–1203.
- Jenkins, R. (1987). "J. D. Hanawalt," *Powder Diffr.* **2**, 266.
- Mereiter, K., and Zemmann, J. (1976). "Neubearbeitung des quecksilberminerals eglestonit: kristall-struktur, chemische zusammensetzung und synthese," *Tschermaks Mineral. Petrog. Mitt.* **23**, 105–115.
- Mereiter, K., Zemmann, J., and Hewat, A. W. (1992). "Eglestonite, $[\text{Hg}_2]_3\text{Cl}_3\text{O}_2\text{H}$: confirmation of the chemical formula by neutron powder diffraction," *Am. Miner.* **77**, 839–842.
- Roberts, A. C., Bonardi, M., Erd, R. C., Criddle, A. J., and LePage, Y. (1991). "Watersite, $\text{Hg}_4^{1+}\text{Hg}^{2+}\text{Cr}^{6+}\text{O}_6$, a new mineral from the Clear Creek claim, San Benito County, California," *Mineral. Rec.* **22**, 269–272.
- Roberts, A. C., Bonardi, M., Erd, R. C., Criddle, A. J., Stanley, C. J., Cressey, G., Angel, R. J., and Laflamme, J. H. G. (1990a). "Edgarbaileite—the first known silicate of mercury, from California and Texas," *Mineral. Rec.* **21**, 215–220.
- Roberts, A. C., Ercit, T. S., Erd, R. C., and Oscarson, R. L. (1990b). "Szymańskiite, $\text{Hg}_{16}^{1+}(\text{Ni,Mg})_6(\text{CO}_3)_{12}(\text{OH})_{12}(\text{H}_3\text{O})_8^{1+} \cdot 3\text{H}_2\text{O}$, a new mineral species from the Clear Creek claim, San Benito County, California," *Can. Mineral.* **28**, 703–707.
- Roberts, A. C., Ercit, T. S., Groat, L. A., Criddle, A. J., Erd, R. C., and Williams, R. S. (1995). "Peterbaylissite, $\text{Hg}_3^{1+}(\text{CO}_3)(\text{OH}) \cdot 2\text{H}_2\text{O}$, a new mineral species from the Clear Creek claim, San Benito County, California," *Can. Mineral.* **33**, 47–53.
- Roberts, A. C., Szymański, J. T., Erd, R. C., Criddle, A. J., and Bonardi, M. (1993). "Deanesmithite, $\text{Hg}_2^{1+}\text{Hg}_3^{2+}\text{Cr}^{6+}\text{O}_5\text{S}_2$, a new mineral species from the Clear Creek claim, San Benito County, California," *Can. Mineral.* **31**, 787–793.
- Šćavničar, S. (1956). "The crystal structure of oxy-mercuric-mercurous chloride, $2\text{HgO} \cdot \text{Hg}_2\text{Cl}_2$," *Acta Cryst.* **9**, 956–959.
- Szymański, J. T., and Roberts, A. C. (1990). "The crystal structure of szymańskiite, a partly disordered $(\text{Hg}-\text{Hg})^{2+}$, (Ni,Mg) hydronium-carbonate-hydroxide-hydrate," *Can. Mineral.* **28**, 709–718.
- Vasiliev, V. I., Lavrentiev, Yu. G., and Paltchik, N. A. (1981). "Poyarkovite, Hg_3ClO —a new natural oxide-chloride of mercury," *Zap. Vses. Miner. Obshch.* **110**, 501–505.