

**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<sup>1</sup>**

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ABSTRACT

Peterbaylissite, idealized as  $\text{Hg}_3^{1+}(\text{CO}_3)(\text{OH})\cdot 2\text{H}_2\text{O}$ , is orthorhombic, space group *Pcab* (61), with unit-cell parameters refined from powder data: *a* 11.130(2), *b* 11.139(3), *c* 10.725(3) Å, *V* 1330(1) Å<sup>3</sup>, *a:b:c* = 0.9992:1:0.9628, *Z* = 8. The strongest six reflections in the X-ray powder pattern [*d* in Å(*l*)(*hkl*)] are: 4.84(50)(012), 2.969(70)(231), 2.786(70)(040,400), 2.648(100)(223), 2.419(60)(241,024,412), and 1.580(50)(623). 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. The mineral is most closely associated with ferroan magnesiochromite and is found as isolated and clustered grains on a crust composed of ferroan magnesite and quartz. Other mercury-bearing phases found on the holotype specimen include cinnabar, metacinnabar and native mercury. Individual crystals of peterbaylissite range in size from 20 µm up to 0.2 mm, but the average length of crystals is approximately 0.1 mm. Crystals are subhedral to euhedral, elongate [001], and possess a wedge-like shape with a conchoidal outline. Platy crystals also are present but are rare. The mineral is opaque, black to very dark red-brown color, with a dark brown-black streak. Physical properties include: submetallic to adamantine luster, irregular fracture, brittle, nonfluorescent, hardness less than 5, calculated density 7.14 g/cm<sup>3</sup> (for both the empirical and idealized formulae). In polished section, peterbaylissite is weakly to moderately birefractant and is nonpleochroic. In reflected plane-polarized light, it is grey with a slight blue tinge and possesses abundant orange and brilliant yellow-white internal reflections. The anisotropy is weak, with dull and dark grey and brown rotation tints. Measured values of reflectance for two grains, in air and in oil, are tabulated. Electron-microprobe analyses yielded Hg<sub>2</sub>O 87.4(1.5) wt.%. The empirical formula, derived from crystal-structure analysis and electron-microprobe analyses, is  $\text{Hg}_{3.00}^{1+}(\text{CO}_3)(\text{OH})\cdot 2\text{H}_2\text{O}$ , based on O = 6. The idealized formula requires Hg<sub>2</sub>O 87.54, CO<sub>2</sub> 6.16, H<sub>2</sub>O 6.30, total 100.00 wt.%. Important features of the crystal structure are summarized. This is the first natural occurrence of Hg<sup>1+</sup> as an isolated ion in an oxysalt. The mineral is named for Professor Emeritus Peter Bayliss, University of Calgary, for his many important contributions to structural and experimental mineralogy, and for his long-standing service to the International Centre for Diffraction Data.

*Keywords:* peterbaylissite, new mineral species, hydrated mercurous hydroxide-carbonate, X-ray data, electron-microprobe data, reflectance data, infrared-absorption data, Clear Creek mine, San Benito County, California.

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## SOMMAIRE

La peterbaylissite, dont la composition idéale est  $\text{Hg}_3^+(\text{CO}_3)(\text{OH})\cdot 2\text{H}_2\text{O}$ , est orthorhombique, groupe spatial *Pcab* (61), avec les paramètres réticulaires suivants, affinés à partir du spectre de diffraction sur poudre:  $a$  11.130(2),  $b$  11.139(3),  $c$  10.725(3) Å,  $V$  1330(1) Å<sup>3</sup>,  $a:b:c = 0.9992:1:0.9628$ ,  $Z = 8$ . Les six raies les plus intenses du spectre de diffraction [ $d$  en Å( $hkl$ )] sont: 4.84(50)(012), 2.969(70)(231), 2.786(70)(040,400), 2.648(100)(223), 2.419(60)(241,024,412), et 1.580(50)(623). Il s'agit d'un minéral rarissime d'un petit indice de prospection près de la mine de mercure de Clear Creek, dans le district de New Idria, comté de San Benito, Californie, abandonnée depuis fort longtemps. La peterbaylissite y est étroitement associée à la magnésiochromite ferreuse, et s'y présente sous forme de grains isolés ou en amas sur une croûte de magnésite ferreuse et de quartz. Les autres minéraux contenant du mercure qui coexistent sur l'échantillon holotype sont cinabre, métacinabre et mercure natif. Les cristaux individuels vont de 20 µm à 0.2 mm (0.1 mm de longueur en moyenne). Ils sont sub-idiomorphes ou idiomorphes, allongés sur [001], en biseau et à fracture conchoïdale; les cristaux en plaquette sont rares. La peterbaylissite est opaque, noire à rouge-brun très foncé, avec rayure brun-noir foncé. L'éclat est sub-métallique à adamantin, et la cassure, irrégulière. C'est un minéral cassant, non-fluorescent, d'une dureté inférieure à 5. La densité calculée est 7.14, à la fois pour la formule empirique et idéalisée. Dans les sections polies, elle montre une biréflectance faible ou modérée; elle n'a aucun pléochroïsme. En lumière réfléchie polarisée en plan, elle est grise avec une teinte bleuâtre, et montre une profusion de réflexions internes de couleur orange et jaune-blanc intense. L'anisotropie est faible, avec des teintes de rotation ternes, du gris foncé au brun. Nous présentons les valeurs mesurées de la réflectance pour deux grains, dans l'air et dans l'huile. Les analyses à la microsonde électronique ont donné 87.4(1.5)% de  $\text{Hg}_2\text{O}$  (poids). La formule empirique, dérivée de l'ébauche de la structure cristalline et des résultats des analyses à la microsonde électronique, serait  $\text{Hg}_{3.00}^+(\text{CO}_3)(\text{OH})\cdot 2\text{H}_2\text{O}$ , sur une base de six atomes d'oxygène. La formule idéalisée requiert  $\text{Hg}_2\text{O}$  87.54,  $\text{CO}_2$  6.16,  $\text{H}_2\text{O}$  6.30, total 100.00 (poids). Nous présentons les faits saillants de la trame cristalline. Il s'agit du premier exemple d'un oxy sel naturel contenant le  $\text{Hg}^{+2}$  isolé. Le nom honore le professeur émérite Peter Bayliss, de l'Université de Calgary, pour ses nombreuses contributions importantes à la minéralogie structurale et expérimentale, et son implication soutenue dans les activités du International Centre for Diffraction Data.

(Traduit par la Rédaction)

**Mots-clés:** peterbaylissite, nouvelle espèce minérale, hydroxyde-carbonate mercurieux hydraté, données de diffraction X, données de microsonde électronique, réflectance, spectre d'absorption infra-rouge, mine de Clear Creek, comté de San Benito, Californie.

## INTRODUCTION

The new mineral species described here, peterbaylissite, was first identified, both by X-ray powder diffraction and by X-ray single-crystal analysis, in 1985 by one of us (RCE). The rock specimen that was eventually found to contain the mineral had been originally collected in 1960 by amateur mineralogist Mr. Edward H. Oyler, 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 mineral superficially resembles both specular hematite and the locally ubiquitous magnésiochromite, and thus was not positively identified as a potential new mineral species until subjected to routine X-ray powder-diffraction study. Despite assiduous searches at the prospect pit over the course of a number of years, only one specimen containing crystals of peterbaylissite has so far been found.

The mineral is named *peterbaylissite* in honor of Dr. Peter Bayliss, professor emeritus of mineralogy, Department of Geology and Geophysics, University of Calgary, Calgary, Alberta. Dr. Bayliss has made many significant contributions to the science of both structural and experimental mineralogy and has devoted much time and energy to the International Centre for Diffraction Data, publisher of the Powder Diffraction

File. In particular, he has concentrated his efforts to substantially improve the X-ray powder-diffraction file for minerals. In addition, he was chairman of the Commission on Classification of Minerals, IMA. The mineral and mineral name have been approved by the Commission on New Minerals and Mineral Names, IMA. The holotype specimen is preserved within the Systematic Reference Series of the National Mineral Collection at the Geological Survey of Canada, Ottawa, under catalogue number NMC 67533. A polished section containing several grains of peterbaylissite used for both electron-microprobe and reflectance studies, is preserved at The Natural History Museum, London, Great Britain as BM 1993, 431, and polished mount E.1492.

## OCCURRENCE AND ASSOCIATED MINERALS

Peterbaylissite is an extremely rare constituent at the Clear Creek claim. Only one peterbaylissite-bearing area, measuring 15 × 10 mm, on a single specimen has been identified to date. Within this area, the crystals of peterbaylissite are isolated and clustered on a yellow-brown crust composed of ferroan magnésite and quartz. They are intimately associated with grains of ferroan magnésiochromite that are macroscopically similar in color but are substantially larger in size. The host rock, which is an altered

serpentinite, is composed of quartz, chalcedony, opal, magnesite, goethite, ferroan magnesiochromite, and minor chlorite and dolomite. Associated mercury-bearing minerals on this holotype specimen are cinnabar, metacinnabar and native mercury. Other mercury-bearing minerals identified by X-ray-diffraction analyses from the Clear Creek claim include edgarbaileyite (Roberts *et al.* 1990a, Angel *et al.* 1990), szymańskiite (Roberts *et al.* 1990b, Szymański & Roberts 1990), wattersite (Roberts *et al.* 1991), deansmithite (Roberts *et al.* 1993), edoylerite (Erd *et al.* 1993), eglestonite, calomel, terlinguaite, mosesite, gianellaite, montroydite, and five unnamed mercury-bearing phases that are currently under investigation. A description of the geology of the Clear Creek mercury mine is given by Eckel & 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 edoylerite (Erd *et al.* 1993). Peterbaylissite probably formed as an alteration product of pre-existing mercury-bearing minerals such as cinnabar.

#### PHYSICAL PROPERTIES

Peterbaylissite occurs as isolated or clustered crystals on a secondary yellow-brown crust composed of ferroan magnesite and quartz. Individual crystals range in size from 20  $\mu\text{m}$  up to 0.2 mm; the average size is approximately 0.1 mm in longest dimension. Crystals are subhedral to euhedral, are somewhat elongate [001], and possess a wedge-like shape with an outline similar to that of a slightly deformed tear drop. A few rare platy crystals also are present. No obvious crystal forms were observed. The mineral is opaque, black to very dark red-brown in color, with a dark brown-black streak. It possesses a submetallic to adamantine luster, an irregular fracture, is brittle, and is nonfluorescent under both long- and short-wave ultraviolet radiation. Neither cleavage nor twinning was observed. The crystals are too small for an accurate determination of hardness (although the hardness is definitely less than 5, as the mineral is easily scratched with a needle), and there is insufficient material available for a determination of density using the Berman balance. In any case, since many grains contain microveinlets of ferroan magnesite, a measured specific gravity would, most probably, give a result that is anomalously low. Peterbaylissite turns colorless and becomes transparent in cold concentrated HCl, but does not appear to effervesce. The mineral seems to be unaffected in both cold dilute HCl and cold concentrated  $\text{H}_2\text{SO}_4$ .

#### X-RAY STUDIES

Two crystals of peterbaylissite, one mounted with  $c^*$  and the other mounted with  $b^*$  parallel to the dial

axis, were examined by single-crystal precession methods employing Zr-filtered  $\text{MoK}\alpha$  radiation. The following levels were collected:  $hk0 \rightarrow hk3$ ,  $0kl \rightarrow 3kl$ ,  $h0l \rightarrow h3l$ ,  $10l^*Ab^*$  and  $110^*Ac^*$ . The mineral is pseudotetragonal, but precession films indicate orthorhombic symmetry, and measured unit-cell parameters  $a$  11.12,  $b$  11.13, and  $c$  10.70 Å. The position and intensity of nodes along the  $a^*$  and  $b^*$  axes of  $hk0$  photographs are different:  $h00$  with  $h = 4n$  only present;  $0k0$  with  $k = 2n$  only present. The systematic absences ( $0kl$  with  $l \neq 2n$ ;  $h0l$  with  $h \neq 2n$ , and  $hk0$  with  $k \neq 2n$ ) dictate that the space group is uniquely defined as  $Pcab$  (61). The symmetry and space group have been confirmed by the results of a crystal-structure analysis (Ercit *et al.*, in prep.). The refined unit-cell parameters,  $a$  11.130(2),  $b$  11.139(3),  $c$  10.725 (3) Å,  $V$  1330(1) Å<sup>3</sup> and  $a:b:c = 0.9992:1:0.9628$ , are based on the  $d$  values of 19 X-ray powder lines between 2.969 and 1.373 Å for which unambiguous indexing was possible, based on visual inspection of single-crystal precession films. A fully indexed powder pattern is presented in Table 1. The powder data are unique and bear no resemblance to any other inorganic phase listed in the Powder Diffraction File. With  $Z = 8$ , the calculated density for  $\text{Hg}_3^{1+}(\text{CO}_3)(\text{OH})\cdot 2\text{H}_2\text{O}$  is 7.14 g/cm<sup>3</sup>.

#### Summary of structural features

Peterbaylissite has four cation sites; three of these are occupied by Hg atoms, and one by a C atom. This C atom is triangularly coordinated by oxygen atoms O1, O2 and O3, as is expected for carbonate groups. Mercury atoms Hg1, Hg2 and Hg3 are each linearly coordinated by oxygen atom O3 and by OH. The O atoms that make up the two water molecules, OW1 and OW2, are each weakly bonded to all Hg atoms. Peterbaylissite possesses a sheet structure. The linkage of Hg, O and OH atoms results in puckered hexagonal sheets; Hg atoms are located along the edges of the hexagons, with O and OH atoms located at the corners. Carbonate groups, water molecules and weak Hg–O interactions serve to reinforce bonding between adjacent sheets. The structure is unique for the occurrence of mercury as an isolated  $\text{Hg}^{1+}$  ion in an oxysalt, rather than as the mercurous ion  $\text{Hg}_2^{2+}$ . A comprehensive report on this unique structure will be published elsewhere (Ercit *et al.*, in prep.).

#### OPTICAL PROPERTIES

The polished section of peterbaylissite consists of a compact aggregate of variably sized (5  $\times$  70  $\mu\text{m}$  to 30  $\times$  100  $\mu\text{m}$ ) crystals (or fragments), all of which are irregularly fractured to a greater or lesser extent.

In plane-polarized reflected light, the mineral is grey with a slight blue tinge. It is weakly to moderately birefractant, but is not pleochroic. Brilliant

TABLE 1. X-RAY POWDER-DIFFRACTION DATA FOR PETERBAYLISSITE

<i>I</i> <sub>est.</sub>	<i>d</i> <sub>meas.</sub>	<i>I</i> <sub>calc.</sub>	<i>d</i> <sub>calc.</sub>	<i>hkl</i>	<i>I</i> <sub>est.</sub>	<i>d</i> <sub>meas.</sub>	<i>I</i> <sub>calc.</sub>	<i>d</i> <sub>calc.</sub>	<i>hkl</i>
40	6.35	14	6.35	111	5	1.994	2	2.001	205
30	5.58	13	5.57	020	40	1.969	10	1.968	440
		8	4.98	120	5	1.931	1	1.932	044
40	4.95	27	4.94	201	30	1.903	10	1.902	414
50	4.84	40	4.83	012	3	1.856	2	1.857	060
		6	4.52	121			2	1.832	135
40b	4.48	14	4.52	211			4	1.832	315
		23	4.43	112	30	1.829	2	1.828	601
40	3.87	19	3.86	022			5	1.824	424
10	3.65	4	3.65	122	30	1.787	9	1.788	006
3	3.26	1	3.26	113			9	1.762	235
3	3.175	1	3.173	222	30	1.760	8	1.754	062
		1	3.088	320			1	1.739	540
3	3.076	1	3.053	032	10	1.735	3	1.738	261
5	3.008	8	3.008	203	25	1.713	6	1.714	054
70	2.969	48	2.968	231	5	1.694	2	1.694	154
5	2.908	4	2.904	123	3	1.684	1	1.683	126
		13	2.785	040	20	1.655	7	1.654	452
70	2.786	45	2.783	400	30	1.639	10	1.640	631
5	2.699	3	2.701	140	20	1.624	6	1.625	245
100	2.648	100	2.647	223	50	1.580	20	1.579	623
30	2.607	15	2.607	014			1	1.559	171
10b	2.488	2	2.489	420	10	1.559	1	1.557	711
		29	2.426	241	3	1.545	1	1.544	460
60	2.419	5	2.416	024			6	1.528	641
		13	2.411	412	30	1.528	5	1.526	064
5	2.365	2	2.361	124			3	1.504	046
5	2.334	2	2.337	323	30	1.505	9	1.504	406
30	2.257	11	2.258	422	25	1.483	8	1.484	462
3	2.223	1	2.227	340	25	1.459	6	1.459	454
10	2.181	2	2.181	341	5	1.428	1	1.426	535
		2	2.155	143			1	1.406	723
10	2.144	1	2.141	151	5	1.405	1	1.403	605
		1	2.139	511	15	1.391	4	1.391	800
3	2.106	1	2.116	333	25	1.373	6	1.373	237
		7	2.070	115			1	1.358	554
30	2.064	2	2.067	520	5	1.358	2	1.358	174
		8	2.057	052			5	1.341	281
15	2.024	4	2.022	512	40	1.338	5	1.338	464
							2	1.337	812
							3	1.323	446
					15	1.323	2	1.322	118

- 114.6 mm Debye-Scherrer powder camera
- Cu radiation, Ni filter ( $\lambda$  CuK $\alpha$  1.54178 Å)
- b = broad line
- intensities visually estimated; calculated intensities from crystal-structure determination
- corrected for shrinkage
- indexed on a 11.130, b 11.139, c 10.725 Å.

yellow-white and orange internal reflections are common in color centers and at some crystal margins. Between crossed polars, the mineral is weakly anisotropic in dull and dark grey and brown rotation tints. If immersed in oil ( $n_D = 1.515$ ), it is lead grey in color, but its appearance is otherwise little changed from that observed in air. The internal reflections,

noted in air, are more pronounced in oil: in plane-polarized light, the minute color-centers,  $\leq 1 \mu\text{m}$  in size, remain brilliant, and white to yellow, but between crossed polars, a myriad of exceedingly minute red color-centers become visible and "cloud" most crystals. These could not be entirely avoided in the selection of areas suitable for the measurement of

TABLE 2. REFLECTANCE DATA AND COLOR VALUES FOR PETERBAYLISSITE

lambda nm	R <sub>1</sub>	R <sub>2</sub>	<i>i</i> <sub>m</sub> R <sub>1</sub>	<i>i</i> <sub>m</sub> R <sub>2</sub>
400	12.0	13.2	2.19	2.57
420	11.8	12.8	2.15	2.52
440	11.6	12.5	2.09	2.46
460	11.5	12.3	2.04	2.38
470	11.4	12.15	2.02	2.35
480	11.3	12.1	2.00	2.30
500	11.2	11.9	1.96	2.25
520	11.1	11.7	1.92	2.20
540	11.0	11.65	1.89	2.16
546	10.95	11.6	1.88	2.15
560	10.9	11.5	1.87	2.13
580	10.9	11.5	1.87	2.11
589	10.9	11.5	1.86	2.11
600	10.8	11.4	1.84	2.09
620	10.7	11.3	1.82	2.04
640	10.75	11.2	1.83	2.03
650	10.7	11.2	1.82	2.04
660	10.6	11.2	1.80	2.02
680	10.6	11.2	1.80	2.01
700	10.6	11.15	1.79	2.01

Color values: Illuminant C (6774K)

x	.305	.303	.301	.298
y	.310	.308	.306	.303
YZ	11.0	11.6	1.9	2.2
λ <sub>d</sub>	476	474	474	475
P <sub>e</sub> %	2.7	3.4	4.6	6.0

reflectance; the reflectance data in Table 2 should be regarded as being subject to small incremental errors resulting from the diffuse reflectance component arising from internal reflections.

Reflectance measurements were made on two grains of peterbaylissite with the equipment and

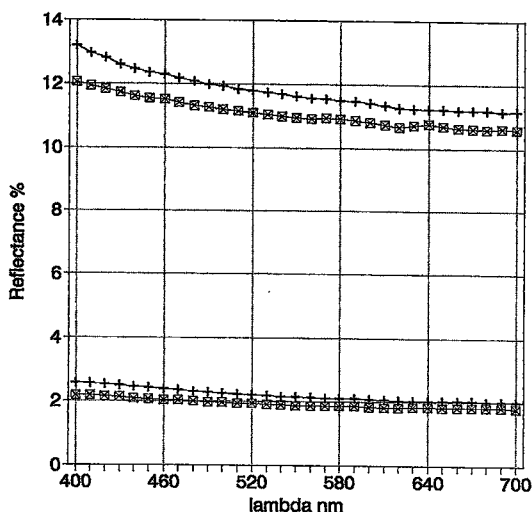


FIG. 1. Reflectance spectra measured in air and in oil ( $N_D$  1.515) for two grains of peterbaylissite.

procedures described by Criddle *et al.* (1983). A Zeiss SiC reflectance standard (no. 472) was used for comparison, and the  $\times 40$  objectives were adjusted to provide effective numerical apertures for measurements of 0.26. The measurements were made on areas  $8 \mu\text{m}$  in diameter. The quantitative data (Table 2, Fig. 1) clearly conform with the description of the mineral in plane-polarized light. Its monotonous normal dispersion, as well as being consistent with its bluish grey appearance, implies that the dispersion of its refringence also is normal, and that it has no absorption bands within the visible spectrum. Indices of refraction at 589 nm, calculated from the reflectance data using the Koenigsberger equations, are in the range 1.98–2.02, for which the corresponding absorption coefficients are about 0.01. Neglecting the calculated absorption, and using the Fresnel equations, the average index of refraction at 589 nm is 2.10.

#### CHEMISTRY

Peterbaylissite crystals were analyzed with a JEOL 733 electron microprobe at the Canadian Museum of Nature, utilizing an operating voltage of 15 kV, a beam current of 7.5 nA, a beam  $4 \mu\text{m}$  in diameter and a 5-second count time. The sample decomposes very quickly under the electron beam, thus necessitating a short count-time. Since only Hg was detected in the energy-dispersion spectra, natural montroydite ( $\text{HgO}$ ) was used as an appropriate mercury standard. Data reduction was performed with a conventional ZAF routine in the Tracor-Northern Task series of programs. The crystal structure was known prior to the interpretation of the analytical data. The average result of two analyses gave  $\text{Hg}_2\text{O}$  87.4(1.5) wt.%. A dearth of pure material prevented the quantitative determination of either  $\text{CO}_2$  or  $\text{H}_2\text{O}$ . Consequently, quantitative values for  $\text{CO}_2$  and  $\text{H}_2\text{O}$  were derived from the results of the crystal-structure analysis (Ercit *et al.*, in prep.). Using these results and the  $\text{Hg}_2\text{O}$  value derived from the electron-microprobe analyses, the chemical formula, based on O = 6, is  $\text{Hg}_{3.00}^{1+}(\text{CO}_3)(\text{OH})\cdot 2\text{H}_2\text{O}$ , identical to the idealized formula. The idealized formula requires  $\text{Hg}_2\text{O}$  87.54,  $\text{CO}_2$  6.16,  $\text{H}_2\text{O}$  6.30, total 100.00 wt.%. This is yet another example of the use of crystal-structure analysis in order to determine the precise chemical formula of a complex mineral species (Hawthorne & Grice 1990). Peterbaylissite is the second reported hydrated  $\text{Hg}^{1+}$ -bearing hydroxyl-carbonate, the first being szymańskiite.

The Gladstone–Dale constants of Mandarino (1981) and the oxide proportions determined from the electron-microprobe data and the crystal-structure refinement lead to a  $K_C$  value of 0.1603 if a Gladstone–Dale constant  $k$  of 0.144 is assumed for  $\text{Hg}_2\text{O}$ , and a  $K_C$  value of 0.1515 if a Gladstone–Dale constant  $k$  of 0.134 is assumed instead.  $K_P$ , calculated using the average index of refraction, 2.10, and the

calculated density, is 0.1541. Thus,  $1-(K_p/K_C)$  ranges from +0.039 to -0.017, depending upon the  $k$  value used for  $\text{Hg}_2\text{O}$ . This indicates an excellent to superior compatibility among the physical and chemical data (Mandarino 1981).

#### INFRARED SPECTROSCOPY

The infrared spectrum of peterbaylissite was obtained using a Spectra-Tech IR-Plan infrared microscope interfaced to a Bomem Michelson MB-120 Fourier-transform infrared spectrometer (FTIR) having a 0.25 mm liquid-nitrogen-cooled mercury cadmium telluride detector. A small amount of pure peterbaylissite was mounted in a diamond anvil microsample cell, then pressure was applied to crush the mineral and cause it to spread as a randomly oriented powder; after crushing, the pressure was released. The diamond cell was then positioned in the microscope accessory and the powdered sample masked so as to isolate a circular area measuring 100  $\mu\text{m}$  in diameter that was between 1 and 5  $\mu\text{m}$  in uniform thickness. Two hundred scans were collected and combined, at 4  $\text{cm}^{-1}$  resolution, from 700 to 4000  $\text{cm}^{-1}$ . The transmittance spectrum (Fig. 2) was produced by taking the ratio of the single-beam spectrum of the specimen in the diamond anvil cell against a single-beam spectrum of the empty diamond anvil cell collected with the same parameters.

The spectrum for peterbaylissite shows the presence of structural water by a shoulder at 1618  $\text{cm}^{-1}$  due to H-O-H flexing. The strong broad absorption band at 3200–3400  $\text{cm}^{-1}$  is due to O-H stretching in  $\text{H}_2\text{O}$

molecules and (OH) groups. Bending of Hg-OH bonds produces the 966  $\text{cm}^{-1}$  band and perhaps some of the weak bands between 1000 and 1200  $\text{cm}^{-1}$ . Internal modes for the carbonate group account for several other strong to medium absorptions ( $\nu_2$  884 and 827,  $\nu_3$  1400–1500,  $\nu_4$  747  $\text{cm}^{-1}$ ). The strong doublet at 1309–1299  $\text{cm}^{-1}$  cannot be assigned with certainty, but may be due to hydrogen bonding between carbonate and hydroxyl. The low frequency of the O-H stretching mode indicates that hydrogen bonding is present.

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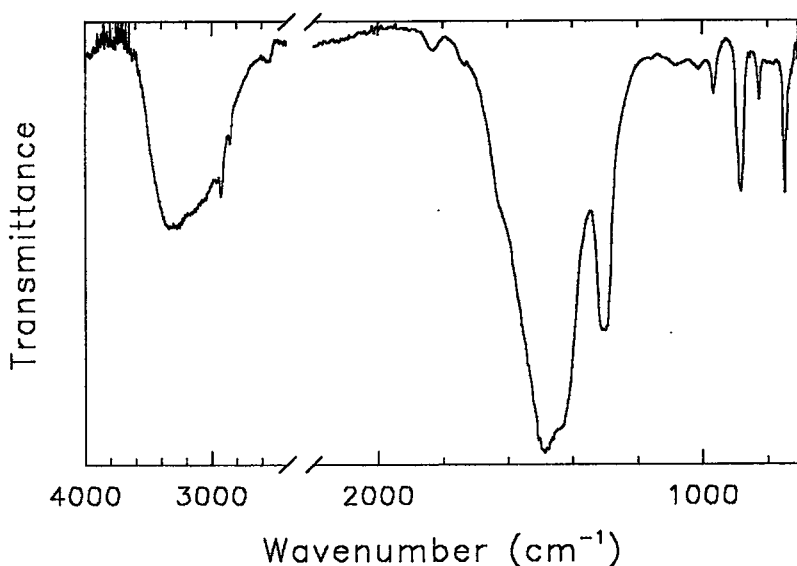


FIG. 2. Infrared-transmission spectrum for peterbaylissite.

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