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DEANESMITHITE, $Hg_2^{1+}Hg_3^{2+}Cr^{6+}O_5S_2$, A NEW MINERAL SPECIES FROM THE CLEAR CREEK CLAIM, SAN BENITO COUNTY, CALIFORNIA[1]

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ABSTRACT

Deanesmithite, idealized as $Hg_2^{1+}Hg_3^{2+}Cr^{6+}O_5S_2$, is triclinic, space group $P\bar{1}$, with unit-cell parameters refined from powder data: *a* 8.116 (6), *b* 9.501 (8), *c* 6.891 (9) Å, α 100.43 (8)°, β 110.24 (8)°, γ 82.80 (8)°, *V* 489 (2) Å^3, *a*:*b*:*c* = 0.8542:1: 0.7253, *Z* = 2. The strongest eight lines in the X-ray powder pattern [*d* in Å(*I*)(*hkl*)] are: 5.72(90)($\bar{1}10$), 3.373(60)($11\bar{2}$,$\bar{1}02$,$\bar{1}21$), 3.008(100)($12\bar{2}$,$21\bar{2}$,$13\bar{1}$,$\bar{1}12$,$\bar{2}02$,$03\bar{1}$), 2.864(50b)(012,201,$\bar{2}20$,$02\bar{2}$), 2.774(50)($\bar{2}21$), 2.536(50)($13\bar{2}$), 2.486(50)(310), and 2.425(60)(221,$03\bar{2}$,$\bar{3}02$). The mineral is a rare constituent in a small prospect pit near the long-abandoned Clear Creek mercury mine, New Idria district, San Benito County, California. It is most closely associated with cinnabar and edoylerite in a host rock principally composed of quartz and magnesite. Deanesmithite typically occurs as fan-shaped aggregates of elongate crystals and, less commonly, as isolated clusters of bladed to acicular radiating crystals. Tabular crystals also are present but rare. The largest known crystal is 0.5 mm in length, but the average crystal length is approximately 0.1 mm. Individual crystals are subhedral to euhedral, with both a bladed and a tabular habit. Crystals are flattened on {100}; bladed crystals are elongate [001]; tabular crystals are elongate [010]; striations on {100} are parallel to [001]; cleavage {$\bar{1}10$} well-developed, {001} fair. Forms observed are: {100}, {320}, {001}, {$\bar{5}10$}, {$01\bar{1}$}, {010}, {210}, {310}, {410}, {510}, {610}, {$\bar{1}10$}, {$\bar{3}20$}, {$\bar{2}10$}, {023}, {$03\bar{2}$}, and {$\bar{1}01$}. The mineral is orange-red with a less intense orange-red streak. Physical properties include: adamantine luster; transparent; nonfluorescent; brittle to friable; irregular to subconchoidal fracture; hardness less than 5; calculated density 8.06 (for empirical formula), 8.14 g/cm^3 (for idealized formula). In polished section, deanesmithite is weakly bireflectant and weakly pleochroic. In reflected plane-polarized light, it is dark bluish grey to light grey with bright yellow-orange to orange-red internal reflections. Measured reflectance values are tabulated, in air and in oil, for two crystals. Electron-microprobe analyses yielded Hg_2O 34.9, HgO 54.4, CrO_3 8.6, S 5.3, sum 103.2, less O=S 2.6, total 100.6 wt.%, corresponding to $Hg^{1+}_{1.98}Hg^{2+}_{2.97}Cr^{6+}_{1.02}O_{5.05}S_{1.95}$ based on O+S=7. The original value for HgO, 90.7 wt.%, was partitioned in a ratio of 2 Hg_2O : 3 HgO after the crystal structure was determined. The crystal structure was solved by direct methods and refined to R = 2.92% from 1748 observed X-ray reflections [$I > 2.5\ \sigma(I)$] out of a total of 2808 unique reflections obtained from measuring and averaging the whole sphere of data to a 2θ of 60° collected with Mo*K*α radiation. Important features of the crystal structure are summarized. The name is for Professor Deane K. Smith, Pennsylvania State University, for his many contributions to structural and experimental mineralogy, and for his long time service to the International Centre for Diffraction Data.

Keywords: deanesmithite, new mineral species, mercurous mercuric chromate sulfide, X-ray data, electron-microprobe data, reflectance data, crystal structure, Clear Creek mine, San Benito County, California.

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SOMMAIRE

La deanesmithite, de formule idéale $Hg_2^{1+}Hg_3^{2+}Cr^{6+}O_5S_2$, est triclinique, groupe spatial $P\bar{1}$, et possède les paramètres réticulaires suivants, affinés à partir du cliché de poudre: a 8.116(6), b 9.501(8), c 6.891(9) Å, α 100.43(8)°, β 110.24(8)°, γ 82.80(8)°, V 489(2) Å^3, a:b:c = 0.8542:1:0.7253, Z = 2. En diffraction X, les huit raies les plus intenses du cliché de poudre [d en Å(I)(hkl)] sont: 5.72(90)($\bar{1}10$), 3.373(60)($11\bar{2},\bar{1}02,\bar{1}21$), 3.008(100)($12\bar{2},21\bar{2},13\bar{1},\bar{1}12,\bar{2}02,03\bar{1}$), 2.864(50b)($012,201,\bar{2}20,02\bar{2}$), 2.774(50)($\bar{2}21$), 2.536(50)($13\bar{2}$), 2.486(50)(310), et 2.425(60)($221,03\bar{2},\bar{3}02$). La deanesmithite est un rare composant d'un petit puit d'exploration près de la mine de mercure de Clear Creek, abandonnée depuis longtemps, dans le district de New Idria, comté de San Benito, en Californie. Elle est étroitement associée à cinabre et édoylerite dans un encaissant de quartz et magnésite. Elle forme typiquement des agrégats en éventail de longs cristaux et, plus rarement, des groupes isolés de cristaux en lames ou en aiguilles disposées en éventail. Les cristaux tabulaires sont plus rares. Les cristaux ont une longueur de 0.1 mm en moyenne, et exceptionnellement, 0.5 mm. Ils sont sub-idiomorphes à idiomorphes, et montrent une forme en lame ou en tablette. Ils sont aplattis sur {100}. Les cristaux en lame sont allongés sur [001]; ceux qui sont tabulaires sont allongés sur [010]. Les stries sur {100} sont parallèles à [001]. Le clivage {$\bar{1}10$} est bien développé, et {001}, médiocre. Nous observons les formes {100}, {320}, {001}, {$\bar{5}10$}, {$01\bar{1}$}, {010}, {210}, {310}, {410}, {510}, {610}, {$\bar{1}10$}, {$\bar{3}20$}, {$\bar{2}10$}, {023}, {$03\bar{2}$}, and {$\bar{1}01$}. C'est un minéral rouge-orange ayant une rayure de couleur plus pâle. Son éclat est adamantin; il est transparent, non fluorescent, cassant, à fracture irrégulière ou sub-concoïdale. Sa dureté est inférieure à 5. Sa densité (calculée) est de 8.06 (formule empirique), et 8.14 (formule idéale). En lumière réfléchie, la deanesmithite est faiblement biréflectante et faiblement pléochroïque; à l'examen en lumière polarisée, elle est gris foncé bleuâtre à gris pâle avec réflexions internes jaune-orange brillant à orange-rouge. La réflectance a été mesurée, dans l'air et dans l'huile, pour deux cristaux. Les analyses à la microsonde électronique ont donné: Hg_2O 34.9, HgO 54.4, CrO_3 8.6, S 5.3, total 103.2, moins O=S 2.6, pour un total de 100.6% en poids, ce qui correspond à la formule $Hg_{1.98}^{1+}Hg_{2.97}^{2+}Cr_{1.02}^{6+}O_{5.05}S_{1.95}$ sur une base de sept anions (O+S). La quantité totale de HgO, 90.7%, a été répartie dans un rapport $2Hg_2O$:3HgO une fois l'ébauche de la structure cristalline terminée. Cette structure a été déterminée par méthodes directes et affinée jusqu'à un R de 2.92% en utilisant 1748 réflexions observées [$I > 2.5\sigma(I)$] des 2808 réflexions uniques obtenues en examinant la sphère entière de données jusqu'à un 2θ de 60° (rayonnement Mo$K\alpha$). Nous présentons les points saillants de la structure. Le nom honore Deane K. Smith, professeur à l'université Pennsylvania State, pour ses nombreuses contributions à la minéralogie structurale et expérimentale, et pour ses nombreuses années de service au International Centre for Diffraction Data.

(Traduit par la Rédaction)

Mots-clés: deanesmithite, nouvelle espèce minérale, sulfure-chromate mercureux et mercurique, données de diffraction X, analyses à la microsonde électronique, données de réflectance, structure cristalline, mine de Clear Creek, comté de San Benito, Californie.

INTRODUCTION

The new mineral species described here, deanesmithite, was first megascopically identified in May 1988 by amateur mineralogist Mr. Edward H. Oyler. The discovery specimen had been collected from a small prospect pit near the long-abandoned Clear Creek mercury mine, New Idria district, San Benito County, California. Mr. Oyler noticed some very small radiating crystals, associated with cinnabar, that appeared to be physically similar to montroydite but were much too reddish in color for that mineral. Routine X-ray powder-diffraction by one of us (RCE) in June 1988 confirmed the mineral's non-identity with montroydite and, as well, showed that the powder data could not be correlated with any known inorganic phase listed in the Powder Diffraction File. In addition, this new mineral also was identified by X-ray powder-diffraction on the type specimen of edoylerite ($Hg_3^{2+}Cr^{6+}O_4S_2$; Erd *et al.* 1993). Sufficient material was then available for a comprehensive mineralogical study and full characterization; the results are reported here. A crystal-structure study is in progress, and partial results also are reported.

The mineral is named *deanesmithite* in honor of Professor Deane K. Smith, College of Earth and Mineral Sciences, Pennsylvania State University, University Park, Pennsylvania. Professor Smith, a native Californian, has made many significant contributions to the science of 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 addition, he is currently editor-in-chief of Powder Diffraction, an international journal dedicated to the characterization of materials. The mineral and mineral name have been approved by the Commission on New Minerals and Mineral Names, I.M.A. The two type specimens are preserved within the Systematic Reference Series of the National Mineral Collection at the Geological Survey of Canada, Ottawa, under catalog numbers NMC 65026 (also type specimen for edoylerite) and 66152.

OCCURRENCE

Deanesmithite has been identified on two specimens collected from a small prospect pit near the long-abandoned Clear Creek mercury mine, New Idria district, San Benito County, California (latitude 36°22′59″N, longitude 120°45′58″W). The mineral must be considered very rare. On the discovery specimen (NMC 66152), it is associated with anhedral crystalline masses of cinnabar and powdery coatings of cinnabar on a rock principally composed of quartz and magnesite. Edgarbaileyite (Roberts *et al.* 1990a, Angel *et al.* 1990) has also been megascopically identified on this specimen. On the type specimen of edoylerite (NMC 65026), deanesmithite is found in vugs and cavities associated with cinnabar and edoylerite. The host rock is composed of quartz, chalcedony, opal, magnesite, goethite, ferroan magnesiochromite, and minor chlorite and dolomite. Other mercury-bearing minerals identified by X-ray diffraction analyses from the Clear Creek claim include szymańskiite (Roberts *et al.* 1990b, Szymański & Roberts 1990), wattersite (Roberts *et al.* 1991), metacinnabar, eglestonite, calomel, terlinguaite, mosesite, gianellaite, montroydite, and four 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). Deanesmithite most likely formed as a result of the reaction between a Cr-rich hydrothermal solution and pre-existing mercury-bearing minerals such as cinnabar.

CRYSTAL MORPHOLOGY

The mineral occurs as fan-shaped elongate prismatic crystal aggregates, up to 0.5 × 0.5 mm in size, and as isolated bladed to acicular radiating clusters of crystals. Tabular crystals also are present but are rare. Individual crystals (Fig. 1) are subhedral to euhedral, and the habit is both bladed and tabular. Crystals are flattened on {100}; bladed crystals are elongate [001], and tabular crystals are elongate [010]. Striations are present on {100} parallel to [001], and there is a well-developed $\{\bar{1}10\}$ cleavage and a fair {001} cleavage. The largest crystal is approximately 0.5 mm in length, but the average length of crystals is approximately 0.1 mm. The length-to-width ratio varies from about 100:1 for acicular crystals to about 20:1 for prismatic crystals. The observed forms, measured by optical goniometry and supported by X-ray single-crystal studies, are: major {100}; minor {320}, {001}, $\{\bar{5}10\}$, $\{01\bar{1}\}$; very small {010}, {210}, {310}, {410}, {510}, {610}, $\{\bar{1}10\}$, $\{\bar{3}20\}$, $\{\bar{2}10\}$, {023}, $\{03\bar{2}\}$, and $\{\bar{1}01\}$. Twinning was not observed megascopically, nor was it found in X-ray single-crystal studies; however, it was observed in reflectance studies.

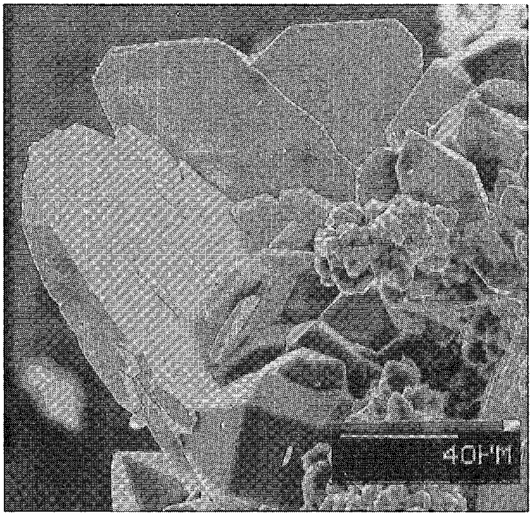

FIG. 1. SEM photomicrograph showing several crystals of deanesmithite protruding from matrix. Scale bar: 40 μm.

PHYSICAL PROPERTIES

Deanesmithite crystals are orange-red and transparent; the streak is the same color but less intense relative to the uncrushed material. The mineral is brittle to friable, possesses an irregular to subconchoidal fracture and an adamantine luster, and is nonfluorescent under both long- and short-wave ultraviolet light. The density could not be measured owing to limitations on size of available specimens and dearth of material; the calculated density based on the empirical formula is 8.06 g/cm^3. The calculated density based on the idealized formula is 8.14 g/cm^3. The hardness is less than 5 (the mineral does not scratch glass), but a more precise value has not been determined.

X-RAY CRYSTALLOGRAPHY

Two crystal fragments, one mounted with b^* and the other mounted with c^* parallel to the dial axis, were examined by single-crystal precession methods employing Zr-filtered Mo radiation. The following levels were photographed: $hk0 \rightarrow hk2$, $0kl \rightarrow 2kl$, $h0l \rightarrow h2l$, $\bar{1}02^* \wedge b^*$, $110^* \wedge c^*$, and $\bar{1}10^* \wedge c^*$. Deanesmithite is triclinic, with space group either $P1$ or $P\bar{1}$ (diffraction aspect P^*). A crystal-structure analysis has shown that the correct space-group is $P\bar{1}$. The reciprocal unit-cell parameters measured and calculated from zero-level precession films are: d_{100} 7.58, d_{010} 9.34, d_{001} 6.39 Å, α^* 81.50°, β^* 70.58°, and γ^* 93.92°.

The X-ray powder-diffraction data are presented in Table 1. The unit-cell parameters were refined using 17 powder reflections representing d values between 3.77 and 1.891 Å for which unambiguous indexing was possible, based on visual inspection of single-crystal precession films. The refined unit-cell parameters are: a 8.116 (6), b 9.501(8), c 6.891(9) Å, α 100.43(8)°, β 110.24(8)°, γ 82.80(8)°, V 489(2) Å^3, and $a:b:c$ = 0.8542:1:0.7253. The powder data are unique and bear no resemblance to any other inorganic phase listed in the Powder Diffraction File.

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

*I*est	*d*Åmeas	*d*Åcalc	*hkl*	*I*est	*d*Åmeas	*d*Åcalc	*hkl*
30	9.33	9.32	010	50	2.774	2.772	$\bar{2}21$
5	6.36	6.39	001	30	2.667	2.670	$31\bar{1}$
30	6.10	6.10	110	15	2.583	2.583	$\bar{1}3\bar{1}$
90	5.72	5.70	$\bar{1}10$	50	2.536	2.533	$13\bar{2}$
40	4.68	4.66	020	50	2.486	2.487	310
40	4.10	4.10	120			2.430	221
5	3.98	3.96	$\bar{1}1\bar{1}$	60	2.425	2.414	$03\bar{2}$
10	3.77	3.78	111			2.412	$\bar{3}02$
30	3.61	3.60	210	5	2.317	2.315	$32\bar{2}$
20	3.52	3.53	021	20	2.185	2.187	$\bar{1}40$
5	3.44	3.44	$\bar{2}10$	30	2.098	2.098	$\bar{2}1\bar{2}$
		3.380	$11\bar{2}$			2.097	$\bar{1}4\bar{1}$
60	3.373	3.373	$\bar{1}02$	20	2.021	2.024	$31\bar{3}$
		3.372	$\bar{1}21$			2.016	$41\bar{1}$
10	3.252	3.246	$22\bar{1}$	5	1.971	1.971	$\bar{2}32$
		3.238	$\bar{1}2\bar{1}$	10	1.927	1.925	132
5	3.170	3.172	$01\bar{2}$	20	1.891	1.890	222
30	3.113	3.108	030	10	1.871	1.872	$\bar{3}13$
5	3.045	3.049	220			1.871	$\bar{2}41$
100	3.008	3.012	$12\bar{2}$	20	1.842	1.843	$\bar{1}4\bar{2}$
		3.011	$21\bar{2}$			1.841	$\bar{4}12$
		3.001	$13\bar{1}$			1.838	023
		2.999	$\bar{1}12$			1.837	$\bar{4}10$
		2.981	$\bar{2}02$				
		2.973	$03\bar{1}$				
30	2.947	2.947	130				
50b	2.864	2.896	012				
		2.874	201				
		2.851	$\bar{2}20$				
		2.840	$02\bar{2}$				

- 114.6 mm Debye-Scherrer powder camera employing Ni-filtered Cu radiation (λ Cu*K*α 1.54178 Å)
- intensities estimated visually; b = broad line
- not corrected for shrinkage and no internal standard used
- indexed on *a* 8.116, *b* 9.501, *c* 6.891 Å, α 100.43°, β 110.24°, γ 82.80°

TABLE 2. REFLECTANCE VALUES* FOR TWO AREAS OF ONE GRAIN OF DEANESMITHITE

Grain:	1		2		1		2	
λnm	R_1	R_2	R_1	R_2	$^{im}R_1$	$^{im}R_2$	$^{im}R_1$	$^{im}R_2$
400	24.8	23.1	25.7	23.2	11.4	10.8	13.7	11.0
10	25.0	23.1	26.0	23.3	11.5	10.9	13.6	11.1
20	25.2	23.1	26.2	23.4	11.5	10.8	13.5	11.2
30	25.15	23.15	26.05	23.45	11.4	10.7	13.0	11.2
40	24.8	23.15	25.7	23.5	11.2	10.7	12.5	11.2
450	24.3	23.2	25.2	23.7	10.8	10.5	11.9	11.2
60	23.8	23.3	24.8	23.8	10.4	10.35	11.25	11.1
70	23.4	23.5	24.2	23.9	10.0	10.3	10.6	10.9
80	22.9	23.6	23.7	24.1	9.61	10.2	10.15	10.8
90	22.5	23.7	23.25	24.2	9.20	10.15	9.69	10.7
500	22.1	23.8	22.8	24.2	8.83	10.1	9.26	10.6
10	21.7	23.7	22.3	24.15	8.50	10.0	8.89	10.4
20	21.3	23.5	22.0	23.9	8.17	9.80	8.60	10.2
30	20.8	23.2	21.7	23.6	7.83	9.49	8.31	9.82
40	20.5	22.9	21.3	23.2	7.61	9.19	8.06	9.52
550	20.3	22.5	20.9	22.8	7.43	8.88	7.85	9.22
60	20.1	22.05	20.65	22.45	7.32	8.61	7.66	8.90
70	20.0	21.8	20.45	22.0	7.32	8.50	7.54	8.68
80	20.0	21.7	20.2	21.7	7.41	8.53	7.46	8.51
90	20.0	21.65	20.1	21.5	7.47	8.60	7.40	8.44
600	20.0	21.55	20.0	21.3	7.54	8.70	7.36	8.38
10	19.9	21.4	19.9	21.2	7.59	8.72	7.33	8.30
20	19.9	21.3	19.8	21.0	7.61	8.70	7.30	8.22
30	19.8	21.15	19.65	20.8	7.60	8.66	7.24	8.15
40	19.7	21.0	19.6	20.7	7.60	8.62	7.21	8.12
650	19.65	20.95	19.4	20.5	7.59	8.56	7.19	8.07
60	19.6	20.8	19.3	20.3	7.54	8.49	7.17	8.00
70	19.45	20.6	19.25	20.2	7.50	8.38	7.14	7.98
80	19.4	20.45	19.2	20.15	7.48	8.33	7.13	7.94
90	19.3	20.4	19.1	20.05	7.46	8.31	7.13	7.96
700	19.25	20.3	19.05	20.0	7.45	8.27	7.12	7.95
Colour values (relative to CIE illuminant C)								
x	0.295	0.302	0.291	0.299	0.283	0.293	0.274	0.285
y	0.296	0.313	0.295	0.313	0.276	0.299	0.268	0.296
Y%	20.6	22.4	21.0	22.6	7.79	9.06	8.02	9.20
λ_d	472	487	476	488	467	478	471	480
P_e%	8.0	3.4	9.3	4.4	14.9	8.2	19.1	11.4

* ^{im}R, N_D 1.515.

OPTICAL PROPERTIES

In transmitted light, deanesmithite is biaxial, with all indices of refraction greater than 2. The direction of the fast ray shows orange-yellow pleochroism, and the direction of the slow ray shows dark reddish orange pleochroism, slow > fast. The optical properties in transmitted light are very difficult to determine because of the high refringence and absorption; therefore, the mineral was studied in reflected light.

Only two grains of deanesmithite were available for optical examination: one, a lath-like crystal (150 × 42 μm), is twinned along its length; the other, also twinned (90 μm across), is a compound intergrowth of smaller (<20 μm) grains, or crystals.

In reflected, plane-polarized light, deanesmithite is weakly bireflectant and weakly pleochroic, from light grey to a slightly darker bluish grey. Yellow-orange internal reflections are common. Between crossed polars, these internal reflections appear orange-red and mask any anisotropic rotation-tints that might be present.

Reflectance measurements (using the equipment and procedures outlined by Criddle *et al.* 1983) were made on both grains relative to a Zeiss SiC reflectance standard (no. 472) with 40× objectives, the effective numerical apertures of which had been adjusted to 0.26. Immersion measurements were made using Zeiss oil, N_D 1.515, at an ambient temperature of 20°C. The samples, which had been polished with diamond abrasives, were lightly buffed with MgO immediately before measurement. As far as could be seen, internal reflections are absent from the areas selected for measurement; however, given the need to measure with high-power objectives (the measured areas were less than 8 μm in diameter), we cannot be absolutely sure that this was the case [*cf.* Dunn *et al.* (1988)]. Further, it should be noted that the optical orientation of the crystals could not be determined, and hence, the reflectance data (though obtained at extinction positions) refer to non-principal directions of vibration.

The reflectance data, and color values calculated from them (relative to CIE Illuminant C) (Table 2) and

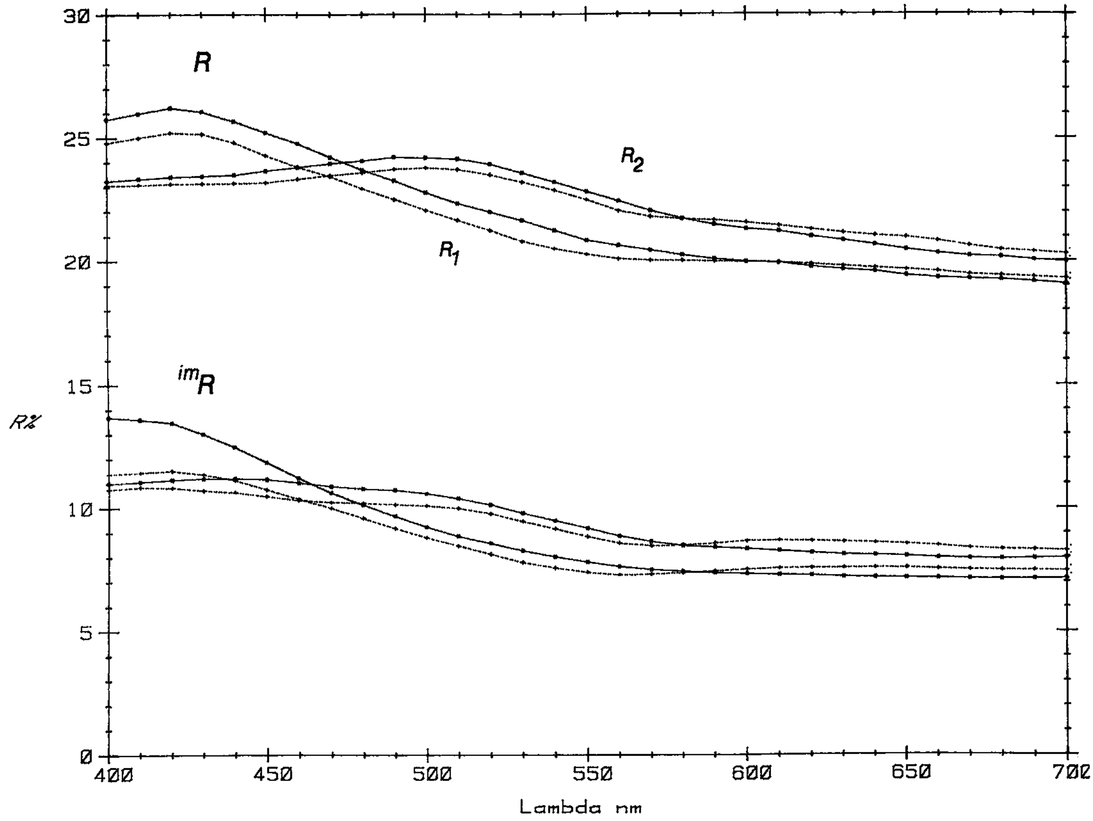

FIG. 2. Reflectance spectra measured in air and in oil (N_D 1.515) for two areas of one grain of deanesmithite.

a graph of the reflectance spectra (Fig. 2), are consistent with the qualitative observations noted above: the reflectance pleochroism is the product of two dispersion curves that are quite different, R_1 corresponding to the lower reflecting and bluer vibration direction for both crystals. If we accept the uncertainty about the optical and crystallographic orientation of the crystals that were measured, it is still evident (from Fig. 2) that the sign of the bireflectance of deanesmithite changes at about 470 nm. Indices of refraction calculated from the R and ^{im}R spectra using the Koenigsberger equations, at 590 nm, are: for n_1, 2.48–2.54, and for n_2, 2.61. The mineral is strongly absorbing at the blue end of the visible spectrum, with absorption coefficients in excess of 1.

CHEMISTRY

Deanesmithite was analyzed with a Cameca SX–50 electron microprobe, with an operating voltage of 20 kV, a beam current of 30 nA, and a slightly defocussed beam 10 µm in diameter. Natural cinnabar (for Hg, S) and synthetic Cr metal (for Cr) were employed as standards. A wavelength-dispersion electron-microprobe scan indicated the absence of all major elements with atomic number greater than 9 other than those reported here. Traces of Fe, Mg, Ni, and Zn were detected, but at levels less than 0.01 wt.%. The average result of six analyses gave HgO 90.7(6), CrO_3 8.6(4), S 5.3(3), sum 104.6, less O=S 2.6, total 102.0 wt.%. In light of preliminary results of a crystal-structure determination (Szymański *et al.*, in prep.), the HgO value was recalculated to Hg_2O and HgO in a ratio of 2:3. This gives Hg_2O 34.9, HgO 54.4, CrO_3 8.6, S 5.3, sum 103.2, less O=S 2.6, total 100.6 wt.%. The valence state of the Cr had originally been assumed to be 6+; the validity of this assumption was confirmed by bond-valence summation derived from results of the crystal-structure analysis. With O+S = 7, the empirical formula is $Hg^{1+}_{1.98}Hg^{2+}_{2.97}Cr^{6+}_{1.02}O_{5.05}S_{1.95}$ or, ideally, $Hg^{1+}_2Hg^{2+}_3Cr^{6+}O_5S_2$, with $Z = 2$. This idealized formula requires Hg_2O 34.79, HgO 54.19, CrO_3 8.34, S 5.35, sum 102.67, less O=S 2.67, total 100.00 wt.%. This is the second reported mercury chromate sulfide (the first is edoylerite).

The mineral is unaffected by cold or hot 1:1 HCl or HNO_3 or by cold aqua regia. However, it is quickly attacked by warm to hot aqua regia, with the formation of gas bubbles and complete conversion to a white material (calomel?).

Summary of Crystal-Structure Results

Inasmuch as details of the crystal structure were found to be essential to arrive at a realistic chemical formula of this species, we report here a summary of the structural results. A paper reporting full details regarding the structure of deanesmithite (Szymański *et al.*) is in preparation.

The structure has been solved and refined to R = 2.92% from 1748 observed X-ray reflections [$I > 2.5\sigma(I)$] out of a total of 2808 unique reflections obtained by measuring and averaging the whole sphere of data, collected with Mo$K\alpha$ radiation to 2θ = 60°. The crystal used for the structure is a small flake, tabular (010), 0.08 mm across and 0.014 mm thick. Empirical absorption corrections (φ sweeps) were applied to the data (maximum : minimum transmission = 5:1). The structure was solved by direct methods, and refined by least-squares using isotropic thermal parameters for oxygen atoms and anisotropic thermal parameters for all other atoms. A secondary extinction correction also was included. Sulfur was identified by its scattering power, about twice that of oxygen.

The crystal symmetry is triclinic, $P\bar{1}$. The least-squares-refined single-crystal unit-cell parameters are: a 8.1287(8), b 9.4916(7), c 6.8940(4) Å, α 100.356(6)°, β 110.163(7)°, γ 82.981(8)°, Z = 2. This is a mixed-valence mercury – disulfide – oxide – chromate mineral, with crystal-chemical formula: $[Hg–Hg]^{2+}\cdot Hg_3^{2+}\cdot Cr^{6+}\cdot S_2\cdot O_5$ or $[Hg–Hg]^{2+}\cdot Hg_3^{2+}\cdot S_2\cdot O\cdot [CrO_4]^{2-}$. The calculated density is 8.125 g/cm³. The "monovalent mercury" is characterized by a typical metal–metal bond of 2.54(1) Å, with one mercury atom bonded to three oxygen atoms (and Hg) in a distorted tetrahedron with three additional oxygen atoms in a second coordination shell. The other monovalent mercury atom is closely linked to a sulfur atom [2.442(4) Å] and to one oxygen atom [2.77(1) Å], and more weakly to five other oxygen atoms at distances between 3.22 and 3.82 Å. Two Hg^{2+} atoms are found at centers of symmetry: 0,0,0 and 1/2,1/2,0. (This accounts for the presence of six mercury atoms in the structure but only five in the formula unit). The first mercury atom has a distorted square-planar coordination: two short bonds at 2.01(1) Å and two longer bonds at 2.84(1) Å. The second mercury atom is roughly octahedrally coordinated, with two opposite bonds to sulfur at 2.352(4) Å and pairs of bonds to oxygen at 2.77(1) and 2.82(1) Å. There are two more Hg^{2+} atoms: the first Hg^{2+} atom has a distorted square-pyramidal coordination, with two sulfur atoms *trans* and three oxygen atoms in the other positions; the second Hg^{2+} atom has a distorted pentagonal dipyramidal coordination, with five oxygen atoms near the plane at distances between 2.55 and 3.44(1) Å, and two sulfur atoms at the apices at 2.364 and 2.359(4) Å. The chromium atom is tetrahedrally bonded to four oxygen atoms at distances between 1.64 and 1.69(1) Å, forming a typical $[CrO_4]^{2-}$ anion. There are no S–O contacts within bonding distance, the closest being at about 3.36 and 3.37 Å to one sulfur atom; to the other, there are no additional atoms within 3.8 Å. This precludes all possibility of oxy-sulfur anions.

Bond-valence summation for the two Hg^{1+} atoms, four Hg^{2+} atoms and one Cr^{6+} atom gives the following values: 0.99, 0.90, 2.18, 1.94, 1.97, 1.98, 5.69 *v.u.*, respectively. For the two sulfur atoms and five oxygen atoms, the values are: 2.05, 2.18, 1.84, 1.89, 1.78, 2.06, 1.78 *v.u.*, respectively. These values are sufficiently close to the theoretical ones as to dispel all doubt about the valences assigned to the individual atoms, and hence the formula of the mineral.

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