

TEDHADLEYITE, $Hg^{2+}Hg^{1+}O_4I_2(Cl,Br)_2$, A NEW MINERAL SPECIES FROM THE CLEAR CREEK CLAIM, SAN BENITO COUNTY, CALIFORNIA

ANDREW C. ROBERTS[§]

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

MARK A. COOPER AND FRANK C. HAWTHORNE

Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada

ALAN J. CRIDDLE[†]

Department of Mineralogy, The Natural History Museum, Cromwell Road, London SW7 5BD, U.K.

JOHN A.R. STIRLING

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

GAIL E. DUNNING

773 Durshire Way, Sunnyvale, California 94087, U.S.A.

ABSTRACT

Tedhadleyite, a new mineral species of ideal composition $Hg^{2+}Hg^{1+}O_4I_2(Cl,Br)_2$, is triclinic, $A\bar{1}$, with unit-cell parameters refined from X-ray powder data: a 7.014(4), b 11.855(6), c 12.601(6) Å, α 115.56(4), β 82.57(4), γ 100.57(4)°, V 927.7(8) Å³, $a:b:c$ 0.5916:1:1.0629, Z = 2. The strongest eight lines of the X-ray powder-diffraction pattern [d in Å(I)(hkl)] are: 5.281(50)(020, $\bar{1}\bar{1}\bar{1}$), 3.143(90)($\bar{1}\bar{3}\bar{1}, \bar{2}\bar{2}\bar{2}$), 3.005(70)($\bar{1}\bar{2}\bar{2}$), 2.981(50)(211), 2.885(100)(113), 2.675(90)($\bar{1}\bar{2}\bar{4}$, $\bar{2}\bar{3}\bar{3}, 131$), 2.508(40)($\bar{2}\bar{1}\bar{3}$) and 1.624(35)(035). The mineral occurs on a single specimen collected from 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 native mercury, calomel and traces of cinnabar, eglestonite and montroydite in a host rock principally composed of quartz and magnesite. Tedhadleyite occurs in a quartz-lined vug as a somewhat elongate spheroidal anhedral mass, 0.3 mm in diameter, which is partly hollow. The mineral is very dark red to black with a red streak. Physical properties include: adamantine to submetallic luster, opaque to translucent (on thin edges), nonfluorescent, poor {010} cleavage, brittle, uneven fracture, hardness less than 3, calculated density 9.43 g/cm³ (for the chemical formula and unit-cell parameters derived from the crystal structure). In polished section, tedhadleyite is very weakly bireflectant, nonpleochroic and moderately anisotropic in shades of grey. In reflected plane-polarized light, it is bluish white with ubiquitous deep red to purplish red internal reflections. Measured reflectance values obtained in air and in oil for a single fragment are tabulated. Averaged and corrected results of electron-microprobe analyses yielded HgO 8.36, Hg_2O 80.50, I 11.11, Cl 2.20, Br 1.62, sum 103.79, less O = I + Cl + Br 1.36, total 102.43 wt.%, corresponding to $Hg^{2+}O_4I_2(Cl,Br)_2$, based on O + I + Cl + Br = 8 *apfu* (atoms per formula unit). The original value for Hg, 85.15 wt.%, was partitioned in a ratio of 1 HgO : 10 Hg_2O after the crystal structure was determined. The mineral name honors Ted A. Hadley of Sunnyvale, California.

Keywords: tedhadleyite, new mineral species, mercurous mercuric oxide iodide chloride bromide, X-ray data, electron-microprobe data, reflectance data, Clear Creek mine, San Benito County, California.

SOMMAIRE

Nous décrivons la tedhadleyite, nouvelle espèce minérale dont la composition idéale serait $Hg^{2+}Hg^{1+}O_4I_2(Cl,Br)_2$. Il s'agit d'un minéral triclinique, $A\bar{1}$, ayant les paramètres réticulaires suivants, affinés à partir du spectre de diffraction sur poudre: a 7.014(4), b 11.855(6), c 12.601(6) Å, α 115.56(4), β 82.57(4), γ 100.57(4)°, V 927.7(8) Å³, $a:b:c$ 0.5916:1:1.0629, Z = 2. Les huit raies les plus intenses du spectre de diffraction obtenu sur poudre [d en Å(I)(hkl)] sont: 5.281(50)(020, $\bar{1}\bar{1}\bar{1}$), 3.143(90)($\bar{1}\bar{3}\bar{1}, \bar{2}\bar{2}\bar{2}$),

[§] E-mail address: aroberts@NRCan.gc.ca

[†] Deceased, May 2002.

3.005(70)($\bar{1}22$), 2.981(50)(211), 2.885(100)(113), 2.675(90)($\bar{1}\bar{2}4$, $\bar{2}\bar{3}3$, 131), 2.508(40)($\bar{2}\bar{1}3$) et 1.624(35)(035). Le minéral a été trouvé sur un seul échantillon prélevé d'un petit puit de prospection près de la mine de mercure Clear Creek, abandonnée depuis fort longtemps, dans le district de New Idria, comté de San Benito, en Californie. Lui sont étroitement associés mercure natif, calomel et des traces de cinnabre, eglestonite et montroydite dans une roche-hôte à quartz + magnésite. La tedhadleyite se présente dans une vacuole tapissée de quartz sous forme de masse allongée, xénomorphe, sphéroïdale, 0.3 mm de diamètre, et partiellement vide. C'est un minéral rouge très foncé à noir, avec une rayure rouge. Parmi les propriétés physiques, notons: éclat adamantin à submétallique, opaque à translucide (sur les bordures minces), nonfluorescent, clivage {010} de piètre qualité, cassant, fracture inégale, dureté inférieure à 3, densité calculée de 9.43 g/cm³ (pour la formule chimique proposée et les paramètres réticulaires dérivés de l'ébauche de la structure). En section polie, la tedhadleyite est très faiblement biréflectante, non pléochroïque et modérément anisotrope en teintes de gris. En lumière réfléchie polarisée, elle est blanc bleuté avec des réflexions internes ubiquistes de rouge foncé à rouge violacé. Les valeurs de réflectance obtenues dans l'air et dans l'huile pour un seul fragment sont présentées. En moyenne, les résultats corrigés d'analyses à la microsonde électronique mènent à HgO 8.36, Hg₂O 80.50, I 11.11, Cl 2.20, Br 1.62, somme 103.79, moins O = I + Cl + Br 1.36, pour un total de 102.43% (poids), correspondant à Hg²⁺_{1.0}Hg¹⁺_{9.8}O_{3.7}I_{2.2}(Cl_{1.6}Br_{0.5})_{2.1}, sur une base de O + I + Cl + Br = 8 atomes par unité formulaire. La valeur originale de la proportion de Hg, 85.15%, a été répartie selon un rapport 1 HgO : 10 Hg₂O suite à l'ébauche de la structure cristalline. Le minéral est nommé en l'honneur de Ted A. Hadley de Sunnyvale, en Californie.

(Traduit par la Rédaction)

Mots-clés: tedhadleyite, nouvelle espèce minérale, oxyde iodure chlorure bromure mercureux mercurique, données de diffraction X, données de microsonde électronique, données de réflectance, mine de Clear Creek, comté de San Benito, Californie.

INTRODUCTION

The new mineral species described here, tedhadleyite, was first identified in the fall of 1996 by the senior author by means of X-ray powder diffraction and by X-ray single-crystal analysis. The rock specimen on which it occurs had originally been collected by one of us (GED) a year or two earlier, 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). Initial scanning electron microscopy (SEM) and energy-dispersion analysis indicated major Hg with subordinate I, Cl and Br, strongly suggestive of a potentially new mercury oxyhalide. A subsequent mineralogical study supported this contention. In fact, this is the first of six new mercury oxyhalides which we hope to fully characterize over the next few years. All must be considered very rare; despite assiduous searches and numerous X-ray powder determinations, only one small tedhadleyite-bearing specimen has so far been found.

The mineral is named *tedhadleyite* in honor of Ted A. Hadley (b. 1961) of Sunnyvale, California. Mr. Hadley helped collect the Hg-bearing samples in which this new mineral was discovered. He is also a past-president of the Bay Area Mineralogists and a long-time collector of minerals, including those at the Clear Creek claim. In addition, he has written numerous software utilities to support mineral collecting and optical mineralogy, and has designed aids for mineral determination. The mineral and mineral name have been approved by the Commission on New Minerals and Mineral Names, IMA (2001–35). Holotype material, consisting of one micromount specimen and a small gelatin capsule containing several tiny fragments of pure tedhadleyite, is housed in the Systematic Reference Series of the National Mineral Collection at the Geological Sur-

vey of Canada, Ottawa, Ontario, under catalogue number NMC68088. The polished section used for both the quantitative reflectance and electron-microprobe studies will be preserved at The Natural History Museum, Great Britain.

OCCURRENCE AND ASSOCIATED MINERALS

Tedhadleyite is an extremely rare constituent at the Clear Creek claim. It has only been identified within one vug on one small micromount specimen (2 × 1.3 × 0.9 cm) that was collected in the mid-1990s. We estimate less than 10 µg of material is available for study. It occurs within a quartz-lined vug in a centimeter-sized quartz vein. Associated minerals found in adjacent vugs are globules of native mercury, greenish calomel and traces of cinnabar, eglestonite and montroydite. The habit of tedhadleyite and the fact that the dominant "grain" is partly hollow would seem to indicate that the mineral formed, *in situ*, as a replacement of native mercury, during a period of high activity of I (with lower Cl and Br) in the fluid or vapor phase. The host rock is a brecciated silica-carbonate rock composed principally of quartz and ferroan magnesite. Other Hg-bearing minerals identified from the Clear Creek claim are listed in Roberts *et al.* (2001) and references therein. Dunning *et al.* (2002) provide a complete description of the history, geology, mineralogy and geochemistry of the Clear Creek claim.

PHYSICAL PROPERTIES

Tedhadleyite occurs as a somewhat elongate spheroidal mass, 0.3 mm in longest dimension, that is partly hollow and has no obvious crystal form. Several very small anhedral masses are situated within the same vug, which measures 2 × 1.5 mm. The mineral is very dark

red to black (similar to wattersite), with a red streak. The main mass is opaque, although thin edges of fragments are translucent. It is brittle, has an uneven fracture and an adamantine to submetallic luster, and is nonfluorescent under both short- and long-wave ultraviolet light. The {010} cleavage is poor. The Mohs hardness is less than 3 (the mineral is easily scratched by a needle), but a more precise value could not be determined. The density could not be measured owing to the dearth of material; the calculated density, on the basis of the chemical formula and unit-cell parameters derived from an investigation of the crystal structure (M.A. Cooper & F.C. Hawthorne, in prep.), is 9.43 g/cm³. Twinning was not observed megascopically or in X-ray single-crystal studies.

X-RAY CRYSTALLOGRAPHY

Single-crystal precession photos of an anhedral fragment of tedhadleyite show that the symmetry is triclinic. The crystal-structure determination (M.A. Cooper & F.C. Hawthorne, in prep.) indicates that $A\bar{1}$ is the correct space-group. The unit-cell parameters, refined from powder data, are for the same orientation as adopted in the structural study.

The unit-cell parameters, a 7.014(4), b 11.855(6), c 12.601(6) Å, α 115.56(4), β 82.57(4), γ 100.57(4) $^\circ$, V 927.7(8) Å³, $a:b:c$ 0.5916:1:1.0629, and $Z = 2$, were refined from 29 powder reflections representing d values between 4.265 and 1.624 Å and for which unambiguous indexing was possible on the basis of the

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

I_{est}	$d \text{ \AA}_{(\text{meas.})}$	$d \text{ \AA}_{(\text{calc.})}$	hkl	I_{est}	$d \text{ \AA}_{(\text{meas.})}$	$d \text{ \AA}_{(\text{calc.})}$	hkl
10	10.19	10.141	0 $\bar{1}1$	*	15	2.430	2.431
5	6.836	6.884	100	*	25	2.368	2.369
30	6.523	6.502	011	*	25	2.334	2.334
20	6.281	6.267	1 $\bar{1}1$	*	10	2.301	2.303
3	5.708	5.675	002		10	2.258	2.260
		5.293	020			2.253	2 $\bar{4}4$
50	5.281	5.257	1 $\bar{1}1$		10	2.227	2.234
10	4.611	4.602	111			2.224	320
5	4.518	4.506	102	3	2.201	2.202	311
		4.505	1 $\bar{2}2$	*	15	2.163	2.162
*	30	4.265	4.262	T02	*	2.108	2.108
*	25	3.939	3.933	120	3	2.080	2.087
*	5	3.854	3.858	0 $\bar{3}1$	15	2.065	2.069
*	30	3.766	3.760	1 $\bar{2}2$		2.064	1 $\bar{2}4$
*	20	3.652	3.649	1 $\bar{3}1$	*	2.036	133
*	5	3.460	3.463	2 $\bar{1}1$	20	1.985	1.987
*	25	3.385	3.385	113		1.980	046
*	25	3.293	3.288	1 $\bar{3}3$		1.957	322
3	3.255	3.251	022		20	1.953	115
			139	T31		1.948	162
90	3.143	3.134	2 $\bar{2}2$	*	10	1.924	1.924
			3.098	0 $\bar{2}4$		1.882	233
20	3.097	3.094	2 $\bar{2}0$		10	1.881	1.871
			3.088	2 $\bar{1}1$		1.854	313
*	70	3.005	3.005	122	10	1.854	1.850
*	50	2.981	2.975	211		1.838	224
5	2.921	2.909	042		5	1.836	1.836
*	100	2.885	2.883	113	*	1.816	1.817
*	20	2.838	2.837	004	*	1.799	1.798
5	2.720	2.714	220		*	1.755	315
			2.683	1 $\bar{2}4$	*	1.715	242
90	2.675	2.675	2 $\bar{3}3$		15	1.690	066
			2.669	131		1.687	411
3	2.639	2.646	040			1.667	057
*	30	2.598	2.597	T40	10	1.664	1.658
*	20	2.541	2.538	144	3	1.643	1.641
*	40	2.508	2.509	2 $\bar{1}3$	*	1.624	1.625
*	5	2.462	2.459	242			035

114.6 mm Debye-Scherrer powder camera employing Ni-filtered Cu radiation (λ Cu $K\alpha$ = 1.54178 Å). Intensities estimated visually. Not corrected for shrinkage and no internal standard used; * = lines used for unit-cell refinement. Indexed on a 7.014(4), b 11.855(6), c 12.601(6) Å, α 115.56(4), β 82.57(4), γ 100.57(4) $^\circ$.

calculated intensities derived from the crystal structure. A fully indexed powder pattern is presented in Table 1. The powder data are not similar to any other inorganic phase listed in the Powder Diffraction File, and no synthetic equivalent is known in the chemical literature.

CHEMICAL COMPOSITION

An anhedral fragment of tedhadleyite, approximately 0.3 mm in longest dimension, was analyzed with a Cameca SX-50 electron microprobe, with an operating voltage of 20 kV, a beam current of 2 nA, a 5-second count time, and a rastered beam. The following standards were used: cinnabar (Hg), iodargyrite (I), halite (Cl) and synthetic KBr (Br). An energy-dispersion spectrum indicated the absence of elements with atomic numbers greater than 9 other than those reported here. The mineral is very unstable under the electron beam; the longer it is subjected to electrons, the higher the Hg value tends to be above the ideal value. The average of seven determinations (and ranges) gave Hg 85.15 (81.58–87.97), I 11.11 (9.95–11.60), Cl 2.20 (1.46–2.83) and Br 1.62 (1.50–1.74) wt.%. The precision of these values is probably average at best owing to the aforementioned instability under the electron beam. After the crystal structure was successfully determined, the Hg value was converted to HgO and then partitioned to HgO and Hg₂O in a 1:10 ratio. This gives HgO 8.36, Hg₂O 80.50, I 11.11, Cl 2.20, Br 1.62, sum 103.79, less O = I + Cl + Br 1.36, total 102.43 wt.%. With O + I + Cl + Br = 8 apfu (atoms per formula unit), the empirical formula is Hg²⁺_{1.0}Hg¹⁺_{9.8}O_{3.7}I_{2.2}(Cl_{1.6}Br_{0.5})_{2.1}. The chemical formula, determined from the structure refinement, Hg²⁺Hg¹⁺₁₀O₄I₂(Cl_{1.16}Br_{0.84})₂, requires HgO 8.23, Hg₂O 79.24, I 9.64, Cl 1.56, Br 2.55, sum 101.22, less O = I + Cl + Br 1.22, total 100.00 wt.%. The crystal-chemical formula of tedhadleyite would not have been successfully unraveled on the basis of chemical composition alone; this is yet another example of the use of crystal-structure analysis to determine the exact chemical formula of a complex mineral species (*cf.* Hawthorne & Grice 1990).

OPTICAL PROPERTIES

In polished section under plane-polarized light, tedhadleyite is bluish white (Fig. 1a), non-pleochroic and not perceptibly bireflectant. Between crossed polars, it is moderately anisotropic, but with monochrome (grey) rotation-tints that are usually masked by red to purplish red internal reflections (Fig. 1b). Reflectance measurements were made in plane-polarized light at positions corresponding to minimum transmission between crossed polars (true extinction being masked by internal reflections). The equipment used included a Zeiss MPM800 micro-spectrophotometer, Zeiss oil and a SiC reflectance standard. The reflectance data are tabulated, together with the calculated color-values

(Table 2); the latter show that the bireflectance averages about 3% absolute, 12.5% relative in air, and that there are only small differences in dominant wavelength between the two directions of measured vibration. These data, and Figure 2, are objective evidence of the perceived appearance of the mineral.

The optical constants, mean index of refraction (*n*) and absorption coefficient (*k*) were calculated from the reflectance data (Fig. 3). The absorptions (the lower two curves) for *R*₁ and *R*₂ are practically inseparable, whereas the indices of refraction differ in much the same way as the *R* curves. It is clear from these values that although tedhadleyite has strong internal reflections in the red to purple range, it is still quite strongly absorbing within the visible spectrum. Too little material was available to allow direct measurement of the absorption and transmission of the mineral. However, recognizing that the MPM800 is the most sensitive instrument available at present, it was decided to attempt to measure the internal reflections between crossed polars. These should be approximately the same as the transmission of the mineral. There are no calibrated standards available for absolute transmission (at least in reflectance mode); thus the comparison was made with the reflectance of SiC. Of course, there is a very substantial absolute difference in value between SiC and the magnitude of the internal reflections of tedhadleyite. However, SiC has the advantage of a nearly constant "grey" or "white" dispersion, and it proved possible to measure the relative spectral dispersion (color) of the transmission of

TABLE 2. REFLECTANCE DATA AND COLOR VALUES FOR TEDHADLEYITE

λ_{nm}	<i>R</i> ₁	<i>R</i> ₂	$^{''}R$ ₁	$^{''}R$ ₂
400	28.25	29.40	14.40	15.30
420	28.00	29.30	14.05	14.90
440	27.60	29.50	13.80	15.05
460	27.40	29.85	13.40	15.35
480	26.70	29.90	12.95	15.30
500	26.20	29.50	12.30	14.90
520	25.35	28.80	11.70	14.20
540	24.60	27.70	11.10	13.50
560	23.85	26.90	10.50	12.70
580	23.10	25.90	10.10	12.00
600	22.60	25.15	9.60	11.40
620	22.20	24.35	9.29	11.00
640	21.80	24.00	9.24	10.80
660	21.50	23.80	9.20	10.70
680	21.15	23.70	9.05	10.60
700	21.05	23.60	9.00	10.50
COM wavelengths:				
470	27.20	30.00	13.20	15.40
546	24.40	27.60	10.95	13.30
589	22.80	25.40	9.83	11.70
650	21.60	23.90	9.24	10.70
CIE Color values: Illuminant C (6774 K)				
<i>x</i>	0.293	0.294	0.281	0.284
<i>y</i>	0.303	0.308	0.290	0.300
<i>y</i> %	24.1	27.0	10.7	12.9
<i>λ_d</i>	480	484	479	483
<i>P</i> %	7.7	6.7	13.35	11.2
Illuminant A (2856 K)				
<i>x</i>	0.431	0.430	0.419	0.420
<i>y</i>	0.404	0.407	0.400	0.405
<i>y</i> %	23.6	26.4	10.4	12.4
<i>λ_d</i>	491	491	490	491
<i>P</i> %	4.1	4.1	7.1	6.7

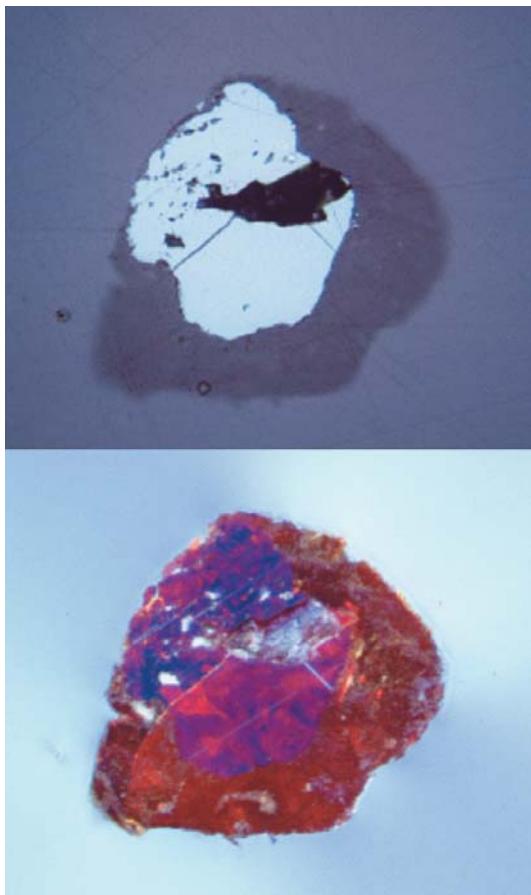


FIG. 1. a. Grain of tedhadleyite in plane-polarized light. b. Same as a. except between crossed polars, showing ubiquitous internal reflections. Horizontal field of view is 0.28 mm.

the mineral (Fig. 4). Color values were calculated from these data: the luminance (transmission) values for R_1 are twice those for R_2 ; the dominant wavelengths for $R_1\lambda_d$ and $R_2\lambda_d$ (for CIE illuminant A) are identical at 616 nm (in the orange-red), and the excitation purity (or saturation) for $R_1P_e\%$ is 63%, and for $R_2P_e\%$, 48%. This procedure offers the possibility of semiquantifying the color of internal reflections for all weakly absorbing (or semi-opaque) minerals, and would be particularly effective if standards were calibrated. This could be done by the measurement of a combination of specular and diffuse reflectance for appropriate minerals or synthetic compounds.

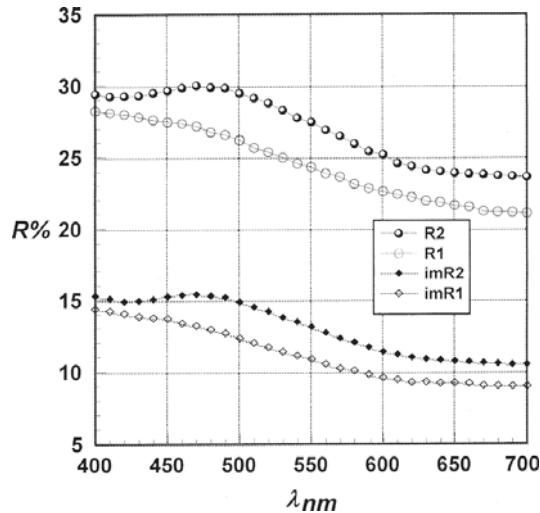


FIG. 2. Reflectance spectra of tedhadleyite measured in air and in oil (N_D 1.515).

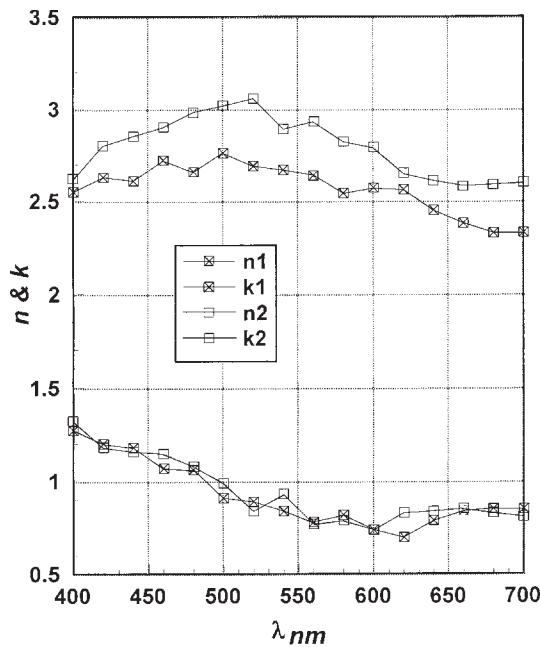


FIG. 3. n and k spectra for tedhadleyite.

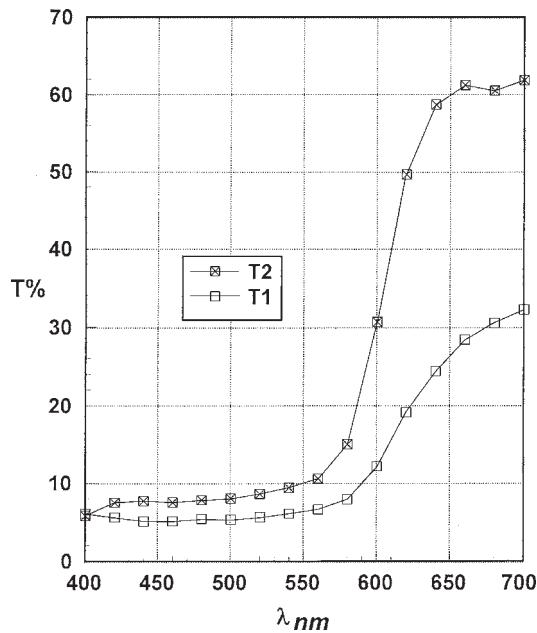


FIG. 4. Transmission spectra for tedhadleyite.

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