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Gatelite-(Ce), a new REE-bearing mineral from Trimouns, French Pyrenees: Crystal structure and polysomatic relationships with epidote and törnebohmite-(Ce)

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ABSTRACT

Gatelite-(Ce), ideally $(Ca_1REE_3)_{\Sigma=4}[Al_2(Al,Mg)(Mg,Fe,Al)]_{\Sigma=4}[Si_2O_7][SiO_4]_3(O,F)\,(OH,O)_2$, is a newly identified mineral from the Trimouns talc deposit, Luzenac, Ariège, French Pyrenees. The mineral occurs as striated colorless crystals finely intergrown with minute lamellae of törnebohmite-(Ce). Associated minerals include pyrite, aeschynite-(Y), dolomite, törnebohmite-(Ce), dissakisite-(Ce), talc, and quartz. Gatelite-(Ce) is insoluble in HCl, relatively hard (Mohs hardness 6–7), brittle with irregular fracture, and exhibits good {100} and imperfect {001} cleavages. Gatelite-(Ce) is monoclinic, space group $P2_1/a$, with the following unit-cell parameters: a = 17.770(4), b = 5.651(1), c =17.458(4) Å, β =116.18(2)°, V = 1573.3(6) Å^3, and Z = 4. The strongest five powder-diffraction lines [d in Å (I/I_o) (hkl)] are 15.67 (87) (001); 3.49 (50) ($\bar{4}12$); 2.97 (100) ($\bar{2}15$); 2.83 (44) (020); and 2.61 (56) ($\bar{6}12$). Electron-microprobe analysis supported by single-crystal structure determination yielded the following empirical formula: $(Ca_{1.09}La_{0.54}Ce_{1.36}Pr_{0.14}Nd_{0.75}Sm_{0.11}Dy_{0.01}Y_{0.04})_{\Sigma 4.04}(Al_{3.06}Mg_{0.51}Fe^{2+}_{0.32}Nb_{0.01})_{\Sigma 3.90}Si_{5.06}O_{20.26}(OH)_{1.60}F_{0.14}$. The calculated density (from the empirical formula) is 4.51 g/cm^3. The structure was solved by direct methods and refined to R_{obs} = 4.65%. It consists of edge-sharing octahedral chains running along the **b** axis, cross-linked by SiO_4 and Si_2O_7 groups. The remaining large cavities are occupied by Ca and REE. The structure of gatelite-(Ce) can be easily described as a regular alternance of slabs of epidote-type structure (E) and slabs of törnebohmite-type structure (T) parallel to the (001) plane. Gatelite-(Ce) can be regarded as a ET polisome within a polysomatic series having epidote and törnebohmite as end-members.

INTRODUCTION

The new mineral species described herein, gatelite-(Ce), is a REE-bearing silicate mineral from the Trimouns talc deposit, Luzenac, Ariège, French Pyrenees, a well-known source of rare minerals, many of them containing rare-earth elements (de Parseval et al. 1997). Although the morphology and chemistry of this mineral resemble those of the epidote-group minerals, gatelite-(Ce) was initially recognized as being a new species, due to its Si and REE content, higher than that required by the crystal-chemical formula of the epidote-group minerals. In addition, the examined material has a significantly different X-ray powder-diffraction pattern.

Gatelite-(Ce) is named in honor of Pierre Gatel, French mineral collector, founder of the Association Française de Microminéralogie. Type-material is housed in the mineralogical collection of the Museum National d'Histoire Naturelle of Paris under the catalogue number MNHM 201.228. The crystal of gatelite-(Ce) used for the structural study is preserved at the Dipartimento di Scienze della Terra, Università di Firenze.

The new mineral and mineral name have been approved by the IMA Commission on New Minerals and Mineral Names (2001-050).

OCCURRENCE AND PHYSICAL PROPERTIES

Gatelite-(Ce) was found in dolomitic levels of the Trimouns talc deposit, Luzenac, Ariège, French Pyrenees. Geological and metallogenic data concerning the talc deposit of Trimouns are summarized by Piret et al. (1990). Associated minerals are: pyrite, aeschynite-(Y), dolomite, törnebohmite-(Ce), dissakisite-(Ce), talc, and quartz. Gatelite-(Ce) formed in the late stages of crystallization like the other REE-bearing minerals in this deposit [trimounsite-(Y), aeschynite-(Y), dissakisite-(Ce)-allanite-(Ce) members, iimoriite-(Y), bastanaesite-group minerals, hingganite-(Y), monazite-(Ce), and xenotime-(Y)].

The mineral occurs as well-formed colorless transparent crystals elongated and striated along [010] (Fig. 1), with vitreous luster. The streak is white. The crystals are made up of minute, oriented intergrowths of gatelite-(Ce) (dark regions in Fig. 2) and törnebohmite-(Ce) (light regions in Fig. 2) with $[010]_{gat}$ parallel to $[010]_{tör}$.

The mineral is insoluble in HCl, relatively hard (Mohs hardness 6–7), brittle with irregular fracture, and exhibits good {100} and imperfect {001} cleavages. Density and optical properties could not be measured, due to the almost constant presence of lamellae of törnebohmite-(Ce) finely intergrown within gatelite-(Ce) and the small size of single-phase grains. On the basis of the chemical composition obtained (see below), the calculated density is 4.51 g/cm^3; a mean refractive index n_{calc} =

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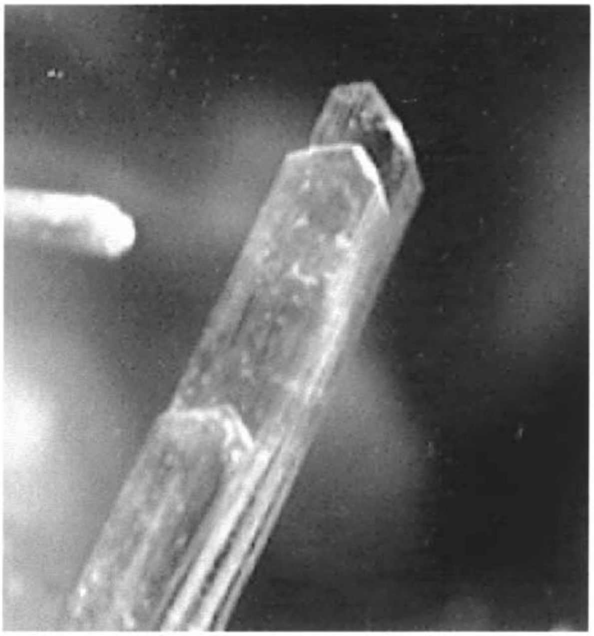

FIGURE 1. Crystals of gatelite-(Ce) from Trimouns (700 μm in length). (Photo R. Vernet)

1.807 was obtained using the Glastone-Dale relationships (Mandarino 1976).

CHEMICAL COMPOSITION

Quantitative chemical analyses were obtained by means of an electron microprobe from a crystal consisting of an intergrowth of gatelite-(Ce) and törnebohmite-(Ce) (Table 1). Other crystals were tested and similar results were obtained. The empirical formula obtained by normalizing to $\Sigma_{cations} = 13.0$ is $(Ca_{1.09}La_{0.54}Ce_{1.36}Pr_{0.14}Nd_{0.75}Sm_{0.11}Dy_{0.01}Y_{0.04})_{\Sigma 4.04}(Al_{3.06}Mg_{0.51}Fe^{2+}_{0.32}Nb_{0.01})_{\Sigma 3.90}Si_{5.06}O_{20.26}(OH)_{1.60}F_{0.14}$. The slight excess of Si and REE cations could be due to the presence of minute lamellae of törnebohmite-(Ce), smaller than the resolution of the instrument. The structure refinement (see below) provides a detailed picture of the cation site-populations and of the OH content and location. H_2O (1.34 wt%) was calculated by the stoichiometry and taking into account crystal-chemical details.

STRUCTURE SOLUTION AND REFINEMENT

Numerous crystals were mounted on an Enraf-Nonius CAD4 single-crystal diffractometer and examined with graphite-monochromatized Mo*K*α X-radiation. Most were found to consist of a fine oriented intergrowth of gatelite-(Ce) and törnebohmite-(Ce), with $\mathbf{b}_{gat} \| \mathbf{b}_{tör}$. A single crystal (30 × 40 × 110 μm, approximately), which did not exhibit any reflections belonging to törnebohmite was selected for the structural study.

Unit-cell dimensions were determined by least-squares refinement of the setting angles of 25 reflections ($10 < \theta_{MoK\alpha} < 17°$). Intensity data were collected ($-28 < h < 28$, $-9 < k < 9$, $0 < l < 28$) in the range $2 < \theta < 35°$, ω-scan mode, with a scan width of 2.5° and a scan speed of 2.35 °/min. Intensities were corrected for Lorentz polarization effects, and for absorption using the semiempirical method of North et al. (1968). Pairs of monoclinic equivalent reflections were averaged (R_{symm} = 3.86%). Systematic absences of $0k0$ ($k = 2n + 1$) and $h0l$ ($h = 2n + 1$) led to the unique choice of the $P2_1/a$ space group. The crystal structure was solved using direct methods in the SHELXS-97 package (Sheldrick 1997) and Fourier syntheses. The positions of most atoms were located on an F_o-Fourier map. The difference-Fourier synthesis calculated with structure factors phased by the contribution of these atoms yielded the position of the remaining O atoms. Structure refinement was performed using SHELXL-93 (Sheldrick 1993). Site-occupancy factors were refined using neutral scattering curves for chemical species at sites where chemical substitutions occur: A1, A2, A3, A4 (Ca vs. Ce), M1 (Mg vs. Fe), M2a, M2b, and M3 (Fe vs. Al). Convergence was rapidly obtained for an anisotropic model of the structure. The difference-Fourier synthesis calculated after the last cycle of refinement revealed the positions of two hydrogen atoms. Using a weighting scheme $w = k/\sigma^2(F_o)$,

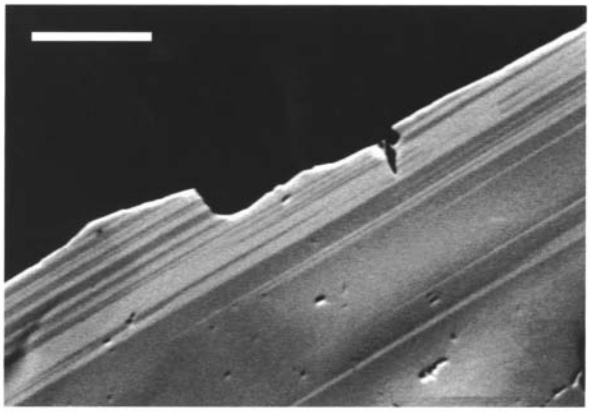

FIGURE 2. BSE image of a crystal of gatelite-(Ce) intergrown with törnebohmite-(Ce). Scale bar is 20 μm.

TABLE 1. Chemical composition of gatelite-(Ce) from Trimouns

	wt%	range		apfu
CaO	5.660	5.01–5.73	Ca	1.091
La_2O_3	8.170	7.97–8.85	La	0.542
Ce_2O_3	20.580	20.20–22.80	Ce	1.356
Pr_2O_3	2.215	2.05–2.62	Pr	0.145
Nd_2O_3	11.740	11.32–12.02	Nd	0.754
Sm_2O_3	1.755	1.53–1.88	Sm	0.109
Dy_2O_3	0.150	0.06–0.30	Dy	0.009
Y_2O_3	0.370	0.21–0.47	Y	0.035
			ΣA sites	4.041
MgO	1.910	1.57–1.98	Mg	0.513
FeO	2.133	2.04–2.15	Fe^{2+}	0.321
Al_2O_3	14.435	13.16–14.58	Al	3.062
Nb_2O_5	0.075	0.00–0.34	Nb	0.006
			ΣM sites	3.902
SiO_2	28.105	26.47–28.51	Si	5.057
F	0.245	0.17–0.55	F	0.139
total	97.543			
–O = F	0.103		Σcations	13.00
Total	97.440			

Note: H_2O not determined; Fe assumed as divalent on the basis of crystal chemical considerations (see text).

the structure refinement converged to a final $R = 4.65\%$ for 4997 reflections with $F_o > 4\sigma(F_o)$, and $R = 7.15\%$ for all 6891 independent reflections. Final atomic coordinates and equivalent isotropic displacement parameters are given in Table 2. Anisotropic displacement parameters are reported in Table 3. The powder diffraction spectrum (Table 4) was calculated from the structural data using XPOW software (Downs et al. 1993). Table 5[1] reports a list of observed and calculated squared structure factors.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

Structure connectivity

The structure of gatelite-(Ce) consists of edge-sharing octahedral chains running along the **b** axis, cross-linked to each other by three non-equivalent SiO_4 isolated tetrahedra and one Si_2O_7 group. The large cavities are occupied by Ca (A1) and REE (A2, A3, and A4). Four independent octahedral sites are present in the structure: M1 octahedra form branched chains with M3 octahedra alternately attached on opposite sides, whereas M2a and M2b octahedra form single chains. Bond distances are reported in Table 6. Figure 3 shows the structure of gatelite-(Ce) projected down the **b** axis.

Modular approach

As shown in Figure 4, the structure of gatelite-(Ce) can easily be described as a regular alternance of modules of epidote-type structure (E) and of törnebohmite-type structure (T). The E modules (dark grey in Fig. 4) are (001) slabs, 10.37 Å thick, with general composition A1 A2 M1 ($M2a_{0.5}$ $M2b_{0.5}$) M3 [Si(1)Si(2)O_7][Si(3)O_4]O(OH). T-type modules (pale grey in Fig. 4) are $(\bar{1}02)$ slabs, 7.08 Å thick, with general composition A3 A4 ($M2a_{0.5}$ $M2b_{0.5}$) [Si(4)O_4 Si(5)O_4] (OH). In this view, the unit-cell dimensions of gatelite-(Ce) can be compared with those of epidote (a = 8.8–9.0, b = 5.6–5.8, c = 10.1–10.2 Å, β = 114–116°; space group $P2_1/m$; Deer et al. 1986) and törnebohmite (a = 7.383, b = 5.673, c = 16.937 Å, β = 112.04°, space group $P2_1/c$; Shen and Moore 1982). In particular: a_{gat} ~

TABLE 2. Fractional atomic coordinates, equivalent isotropic atomic displacement parameters (Å^2) for the crystal structure of gatelite-(Ce)

	x	y	z	U_{eq}
A1	0.36462(9)	0.25491(24)	0.41008(8)	0.0108(2)
A2	0.44606(2)	0.23572(6)	0.25014(2)	0.0075(1)
A3	0.36921(2)	0.28197(7)	0.00984(2)	0.0097(1)
A4	0.03878(2)	0.74136(7)	0.16607(2)	0.0078(1)
M1	0.2497(2)	0.4972(4)	0.5005(2)	0.0102(4)
M2a	0.2400(1)	0.4993(3)	0.2030(1)	0.0058(3)
M2b	0.2402(1)	0.0003(3)	0.2064(1)	0.0057(3)
M3	0.0987(1)	0.7500(3)	0.3769(1)	0.0108(4)
Si1	0.0807(1)	0.2479(3)	0.4765(1)	0.0064(3)
Si2	0.4023(1)	0.7496(3)	0.3350(1)	0.0053(3)
Si3	0.1521(1)	0.2467(3)	0.3127(1)	0.0055(3)
Si4	0.3350(1)	0.7381(3)	0.1031(1)	0.0057(3)
Si5	0.0771(1)	0.2505(3)	0.0772(1)	0.0059(3)
O1a	0.1322(3)	0.4903(8)	0.4807(3)	0.0101(9)
O1b	0.3678(3)	0.5052(9)	0.5211(4)	0.0121(9)
O2a	0.0899(3)	0.4733(9)	0.2904(3)	0.0112(9)
O2b	0.0897(3)	0.0215(9)	0.2893(3)	0.0104(9)
O3a	0.3450(3)	0.9876(8)	0.2993(3)	0.0096(9)
O3b	0.3472(3)	0.5118(8)	0.2954(3)	0.0078(8)
O4	0.2224(3)	0.7471(8)	0.4242(3)	0.0087(8)
O5	0.2258(3)	0.2461(8)	0.4126(3)	0.0094(8)
O6	0.2083(3)	0.2530(8)	0.2587(3)	0.0072(7)
O7	–0.0101(3)	0.2496(9)	0.3976(4)	0.0173(15)
O8	–0.0224(3)	0.7323(9)	0.3100(4)	0.0151(9)
O9	0.4349(3)	0.7400(9)	0.4380(3)	0.0147(10)
O10	0.2789(3)	0.2483(8)	0.1614(3)	0.0072(7)
O11	0.2019(3)	0.7475(8)	0.2490(3)	0.0089(8)
O12	0.2692(3)	0.7544(8)	0.1471(3)	0.0075(7)
O13	0.1347(3)	0.4928(8)	0.1058(3)	0.0089(8)
O14	0.3917(3)	0.9758(8)	0.1246(3)	0.0089(8)
O15	0.2758(3)	0.6711(9)	0.0046(3)	0.0115(9)
O16	0.1335(3)	0.0108(8)	0.1145(3)	0.0091(8)
O17	0.0323(4)	0.2178(9)	-0.0243(3)	0.0234(13)
O18	0.4032(3)	0.5230(8)	0.1411(3)	0.0093(8)
O19	0.0105(3)	0.2753(9)	0.1157(4)	0.0165(10)
H1	0.21(1)	0.75(2)	0.31(1)	0.06(1)
H2	0.25(1)	0.28(2)	0.10(1)	0.04(1)

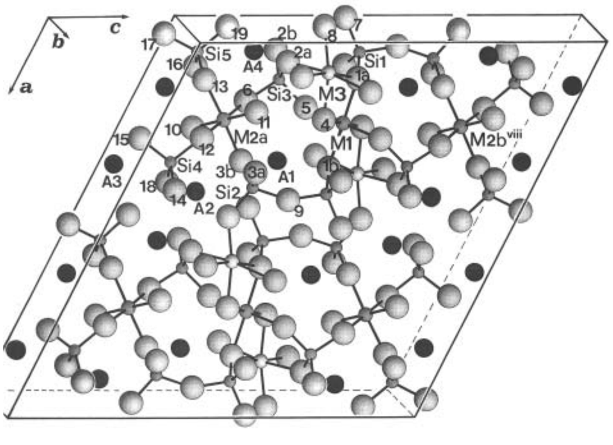

FIGURE 3. Crystal structure of gatelite-(Ce) projected down the **b** axis.

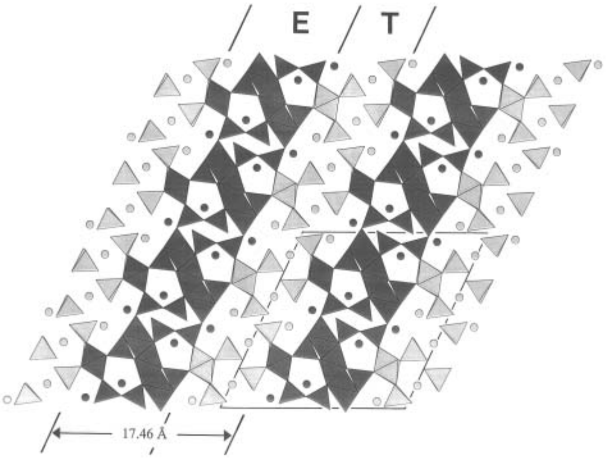

FIGURE 4. Schematic representation of the structure of gatelite-(Ce) in terms of E-type and T-type modules. [010] projection.

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[1] For a copy of Table 5, document item AM-02-020, contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. Deposit items may also be available on the American Mineralogist web site at http://www.minsocam.org.

TABLE 3. Anisotropic displacement parameters (Å^2) for the structure of gatelite-(Ce)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A1	0.0131(5)	0.0103(5)	0.0095(5)	–0.0022(4)	0.0056(4)	0.0022(4)
A2	0.0071(2)	0.0082(2)	0.0060(2)	0.0003(1)	0.0019(1)	0.0001(1)
A3	0.0118(2)	0.0093(2)	0.0057(2)	0.0010(1)	0.0018(1)	0.0004(1)
A4	0.0068(2)	0.0089(2)	0.0062(2)	0.0003(1)	0.0017(1)	0.0003(1)
M1	0.0088(8)	0.0106(9)	0.0103(8)	0.0014(7)	0.0034(7)	0.0016(7)
M2a	0.0052(9)	0.0050(8)	0.0067(8)	0.0006(6)	0.0023(7)	0.0009(6)
M2b	0.0053(9)	0.0049(8)	0.0069(8)	0.0005(6)	0.0028(7)	–0.0005(6)
M3	0.0077(7)	0.0109(7)	0.0148(7)	0.0034(5)	0.0058(5)	0.0045(5)
Si1	0.0052(6)	0.0064(7)	0.0061(6)	0.0003(5)	0.0010(5)	–0.0006(5)
Si2	0.0056(6)	0.0046(7)	0.0058(6)	0.0004(5)	0.0025(5)	–0.0007(5)
Si3	0.0042(6)	0.0069(7)	0.0051(6)	0.0004(5)	0.0018(5)	0.0001(5)
Si4	0.0056(6)	0.0049(7)	0.0064(6)	0.0005(5)	0.0024(5)	0.0001(5)
Si5	0.0061(6)	0.0051(7)	0.0049(6)	–0.0004(5)	0.0009(5)	0.0004(5)
O1a	0.010(2)	0.007(2)	0.014(2)	–0.003(2)	0.005(2)	–0.002(2)
O1b	0.009(2)	0.006(2)	0.022(3)	–0.001(2)	0.008(2)	–0.001(2)
O2a	0.013(2)	0.012(2)	0.011(2)	0.004(2)	0.007(2)	0.001(2)
O2b	0.009(2)	0.013(2)	0.012(2)	–0.003(2)	0.007(2)	–0.003(2)
O3a	0.007(2)	0.006(2)	0.010(2)	–0.002(1)	–0.001(2)	0.001(2)
O3b	0.005(2)	0.009(2)	0.009(2)	–0.004(1)	0.003(2)	–0.001(1)
O4	0.009(2)	0.008(2)	0.009(2)	–0.002(2)	0.003(2)	–0.001(2)
O5	0.008(2)	0.011(2)	0.009(2)	0.002(2)	0.003(2)	0.001(2)
O6	0.006(2)	0.007(2)	0.011(2)	0.001(1)	0.006(2)	0.002(2)
O7	0.006(2)	0.013(2)	0.019(3)	–0.006(2)	–0.007(2)	0.010(2)
O8	0.011(2)	0.020(3)	0.018(2)	0.002(2)	0.010(2)	0.002(2)
O9	0.013(2)	0.027(3)	0.008(2)	-0.001(2)	0.008(2)	0.003(2)
O10	0.008(2)	0.005(2)	0.009(2)	-0.001(1)	0.004(2)	0.002(1)
O11	0.009(2)	0.010(2)	0.008(2)	0.000(2)	0.004(2)	–0.001(2)
O12	0.006(2)	0.009(2)	0.008(2)	0.001(1)	0.003(1)	–0.001(2)
O13	0.009(2)	0.008(2)	0.007(2)	–0.001(2)	0.001(2)	0.001(1)
O14	0.007(2)	0.009(2)	0.011(2)	–0.002(2)	0.005(2)	–0.001(2)
O15	0.012(2)	0.014(2)	0.006(2)	–0.003(2)	0.002(2)	–0.001(2)
O16	0.007(2)	0.006(2)	0.011(2)	0.001(2)	0.001(2)	0.001(2)
O17	0.034(3)	0.021(3)	0.006(2)	–0.014(2)	0.001(2)	–0.001(2)
O18	0.012(2)	0.006(2)	0.009(2)	0.002(2)	0.004(2)	0.002(2)
O19	0.012(2)	0.019(3)	0.023(3)	–0.002(2)	0.012(2)	–0.005(2)

TABLE 4. Calculated powder diffraction data for gatelite-(Ce)

h	k	l	d_{calc}	I/I_{calc}
0	0	1	15.667	87
2	0	0	7.974	27
–2	0	2	7.475	12
–2	1	1	4.764	10
2	0	2	4.655	10
2	1	0	4.611	33
0	1	2	4.583	10
2	1	1	4.146	10
–4	1	2	3.486	50
–2	1	4	3.451	23
4	1	0	3.258	12
4	0	2	3.050	21
–2	1	5	2.967	100
0	2	0	2.826	44
0	1	5	2.740	32
2	2	0	2.663	19
4	0	3	2.654	26
–6	1	2	2.610	56
–6	1	5	2.434	12
–4	2	4	2.254	12
–8	0	2	2.175	15
–4	2	5	2.135	25
4	2	2	2.073	18
4	2	3	1.935	19
6	1	3	1.914	11
2	1	7	1.838	14
–2	3	5	1.657	12
–8	2	7	1.625	13
–6	3	2	1.587	10
0	4	0	1.413	12

Notes: d values calculated on the basis of *a* = 17.770(4), *b* = 5.651(1), *c* = 17.458(4) Å, β = 116.18(2)°. Intensities calculated using XPOW software, version 2.0 (Downs et al. 1993). Only reflections with I/I_{calc} > 10 are listed.

TABLE 6. Selected interatomic distances (Å) together with the refined site-scattering (mean electron number) for gatelite-(Ce) from Trimouns

A1-	O1a(*i*)	2.404(5)	A2-	O2a(*ii*)	2.615(6)
	O1b	2.380(6)		O2b(*ii*)	2.706(5)
	O3a(*ix*)	2.356(5)		O3a(*ix*)	2.700(5)
	O3b	2.380(5)		O3b	2.715(5)
	O5	2.487(5)		O7(*ix*)	2.339(6)
	O6	2.868(5)		O8(*ii*)	2.808(6)
	O7(*ii*)	2.331(6)		O10	2.677(5)
	O9	2.962(6)		O14(*ix*)	2.455(5)
	mean	2.521		O18	2.358(5)
	s.s.	20.0		O19(*ii*)	3.032(6)
				mean	2.641
				s.s.	57.5
A3-	O12(*iii*)	2.763(6)	A4-	O2a	2.468(5)
	O13(*iii*)	2.574(5)		O2b(*v*)	2.497(5)
	O14(*ix*)	2.542(5)		O11	2.607(5)
	O15(*iii*)	2.554(5)		O13	2.751(5)
	O15	2.732(6)		O14(*vii*)	2.682(5)
	O16(*iv*)	2.509(5)		O16(*v*)	2.702(5)
	O17(*iv*)	2.967(7)		O17(*x*)	2.240(5)
	O18	2.500(5)		O18(*vii*)	2.616(5)
	O19(*ii*)	2.394(6)		O19	2.752(6)
	mean	2.615		mean	2.591
	s.s.	56.9		s.s.	56.5
M1-	O1a	1.961(6)	M2a-	O3b	1.877(5)
	O1b	1.967(6)		O6	1.919(5)
	O4(*i*)	1.843(5)		O10	1.860(5)
	O4	1.853(5)		O11	1.884(5)
	O5(*viii*)	1.971(5)		O12	1.936(5)
	O5	1.993(5)		O13	1.892(5)
	mean	1.931		mean	1.895
	λ	1.0055		λ	1.0055
	σ^2	12.52		σ^2	18.49
	s.s.	12.9		s.s.	13.0
M2b-	O3a(*ix*)	1.854(5)	M3-	O1a	2.200(5)
	O6	1.911(5)		O1b(*viii*)	2.161(6)
	O10	1.879(5)		O2a	2.131(5)
	O11(*ix*)	1.872(5)		O2b(*v*)	2.122(6)
	O12(*ix*)	1.934(5)		O4	1.978(5)
	O16	1.868(5)		O8	1.946(6)
	mean	1.886		mean	2.090
	λ	1.0053		λ	1.0337
	σ^2	17.59		σ^2	105.85
	s.s.	13.0		s.s.	17.6
Si1-	O1a	1.631(5)	Si2-	O3a	1.635(5)
	O1b(*i*)	1.639(5)		O3b	1.626(5)
	O7	1.594(5)		O8(*vi*)	1.583(6)
	O9(*i*)	1.635(5)		O9	1.629(5)
	mean	1.625		mean	1.618
	λ	1.0033		λ	1.0013
	σ^2	11.88		σ^2	4.61
Si3-	O2a	1.623(5)	Si4-	O12	1.661(5)
	O2b	1.617(5)		O14	1.621(5)
	O5	1.656(5)		O15	1.616(5)
	O6	1.649(5)		O18	1.636(5)
	mean	1.636		mean	1.633
	λ	1.0068		λ	1.0092
	σ^2	27.22		σ^2	35.42
Si5-	O13	1.649(5)	O10-	O15(*iii*)	2.655(6)
	O16	1.639(5)	O11-	O4	2.916(6)
	O17	1.601(6)			
	O19	1.604(6)			
	mean	1.624			
	λ	1.0028			
	σ^2	9.88			

Note: The mean quadratic elongation (λ) and the angle variance (σ^2) were computed according to Robinson et al. (1971). Symmetry codes are: (*i*) = 1/2 – x, –1/2 + y, 1 – z; (*ii*) = 1/2+ x, 1/2 – y, z; (*iii*) = 1/2 – x, –1/2 + y, -z; (*iv*) = 1/2 – x, 1/2 + y, –z; (*v*) = x, 1 + y, z; (*vi*) = 1/2 + x, 3/2 – y, z; (*vii*) = –1/2 + x, 3/2 – y, z; (*viii*) = 1/2 – x, 1/2 + y, 1 – z; (*ix*) = x, –1 + y, z; *(x)* = –x, 1 – y, –z.

$2a_{\text{epi}} \sim [201]_{\text{tör}}$; $b_{\text{gat}} \sim b_{\text{epi}} \sim b_{\text{tör}}$; $c_{\text{gat}} \sim (c_{\text{epi}} + a_{\text{tör}})$. The doubling of the translation unit along the **a** axis in gatelite-(Ce) is due to distortion away from the mirror symmetry normal to the **b** axis; thus, the space group is $P2_1/a$ instead of $P2_1/m$. Such symmetry deviations are indeed very slight, so the *hkl* ($h = 2n + 1$) reflections are relatively weak. In a similar way, törnebohmite ($P2_1/c$) slightly deviates from $P2_1/m$ symmetry and exhibits *hkl* ($l = 2n + 1$) weak reflections leading to a doubling of the *c* parameter (Shen and Moore 1982).

When repeated indefinitely, E modules and T modules would produce the epidote (Fig. 5) and törnebohmite (Fig. 6) structures, respectively. A regular alternating stacking of E and T modules produces gatelite, which, therefore, can be regarded as an ET polysome within a polysomatic series having epidote and törnebohmite as end members. It is worth pointing out that E and T modules can fit together in any order, so that other sequences can be expected to be discovered; in fact, the E-T interface does not involve significant distortion of the structure and, therefore, chemically-controlled faulted or disordered sequences might be energetically possible.

Cation distribution

A-polyhedra. Cations occupying the A sites can be described as 8-fold (A1), 9-fold (A3 and A4) and 10-fold (A2) coordinated, with distances ranging from 2.33 to 3.03 Å (Table 6). Ca is almost completely ordered at A1, whereas A2, A3, and A4 are filled mainly by REE.

M-octahedra. Crystal chemical details of the octahedral framework of gatelite-(Ce) closely resemble those of the homologous sites in the structure of epidote (Dollase 1971; Gabe et al. 1973; Carbonin and Molin 1980; Bonazzi and Menchetti 1995) and törnebohmite (Shen and Moore 1982), respectively. As in epidote, the M3 octahedron, attached on alternate sides of the M1 octahedral chain, is the largest and most distorted in the structure. The M2a-M2b single chain is quite similar to those observed in epidote (M2) and in törnebohmite (Al). The <M2a-O> (1.895 Å) and the <M2b-O> (1.886 Å) distances are consistent with the assumption of full occupancy by Al, while the <M1-O> distance (1.931 Å) is slightly greater than those observed in epidotes when M1 is completely filled by Al. This could be due to small amounts of Mg substituting for Al at this site. In fact, considering the mean bond distance as a weighted mean of $\langle\text{Mg-O}\rangle_{\text{M1}}$ [2.028 Å in dollaseite-(Ce), Peacor and Dunn 1988] and $\langle\text{Al-O}\rangle_{\text{M1}}$ (1.907 Å in clinozoisites, Bonazzi and Menchetti 1995), a site population of 0.80 Al^{3+} + 0.20 Mg can be assumed. Taking into account the site population assigned to M1, M2a, and M2b, together with the chemical data and the refined occupancy factor (17.6 e^-) for M3, a cation population of approximately 0.33 Al + 0.33 Fe + 0.33 Mg + 0.01 Nb can be estimated. This result may be discussed by comparing the expected <M3-O> value calculated using the end-member <M3-O> distances derived from known interatomic distances for members of the epidote group. These distances were assumed as following: $\langle\text{Al-O}\rangle_{\text{M3}}$ = 1.968 Å, $\langle\text{Fe}^{3+}\text{-O}\rangle_{\text{M3}}$ = 2.055 Å and $\langle\text{Fe}^{2+}\text{-O}\rangle_{\text{M3}}$ = 2.175 Å using the data published by Bonazzi and Menchetti (1995); <Mg-O> = 2.124 Å was then extrapolated assuming a cation population of 0.87 Mg + 0.13 Fe^{2+} at M3 in dollaseite-(Ce) (Peacor and Dunn 1988). An excellent agreement between the observed (2.090 Å) and the predicted value (2.089 Å) is obtained when a site population of 0.333 Al + 0.333 Mg + 0.333 Fe^{2+} is assumed. On the contrary, the value calculated assuming iron as Fe^{3+} (2.049 Å) does not match the observed distance. For this reason, the iron in gatelite-(Ce) was assumed to be divalent.

Si-tetrahedra. The Si1 and Si2 tetrahedra, linked together to form a Si_2O_7 group, as well as the Si3 tetrahedron, are quite

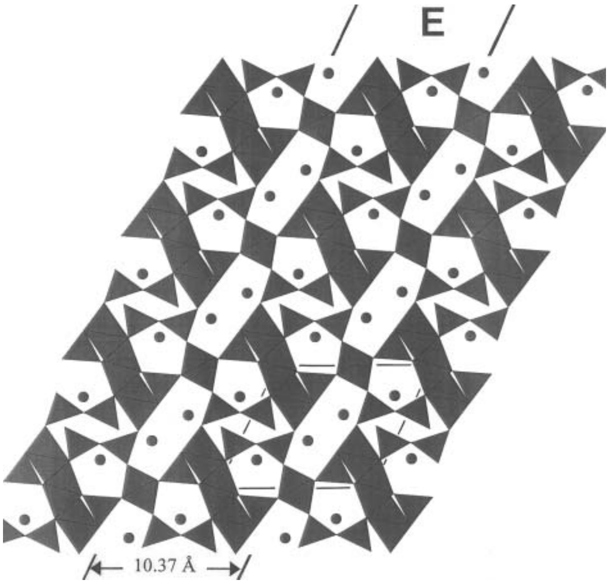

FIGURE 5. Schematic representation of the structure of epidote. Module E is indicated. [010] projection.

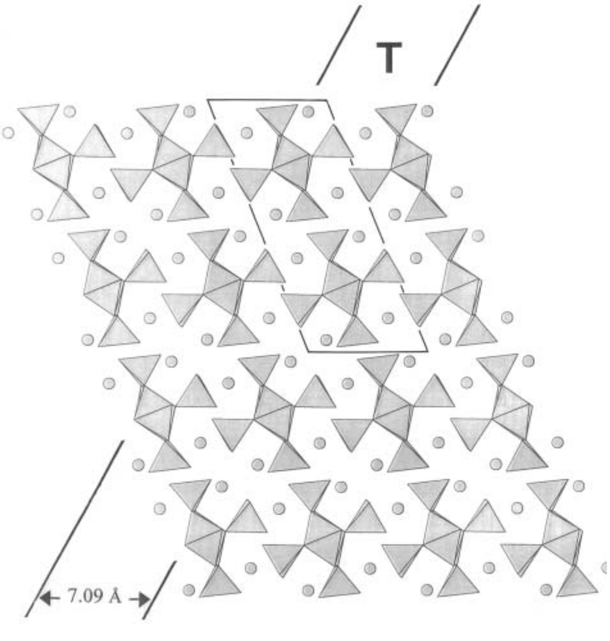

FIGURE 6. Schematic representation of the structure of törnebohmite. Module T is indicated. [010] projection.

TABLE 7. Empirical bond-valence balance for gatelite-(Ce)

	A1	A2	A3	A4	M1	M2a	M2b	M3	Si1	Si2	Si3	Si4	Si5	
O1a	0.307				0.443			0.255	0.981					1.99
O1b	0.328				0.436			0.284	0.960					2.01
O2a		0.282		0.417				0.309			1.003			2.01
O2b		0.222		0.385				0.317			1.019			1.94
O3a	0.349	0.225					0.578			0.971				2.12
O3b	0.328	0.217				0.543				0.995				2.08
O4					1.202			0.466						1.67
O5	0.245				0.838						0.917			2.00
O6	0.088					0.485	0.495				0.935			2.00
O7	0.374	0.596							1.084					2.05
O8		0.168						0.509		1.117				1.79
O9	0.068								0.971	0.987				2.03
O10		0.239				0.568	0.540							1.35
O11				0.286		0.533	0.550							1.37
O12			0.188			0.463	0.465					0.905		2.02
O13			0.314	0.194		0.521							0.935	1.96
O14		0.436	0.342	0.233								1.008		2.02
O15			0.536									1.022		1.56
O16			0.374	0.222			0.556						0.960	2.11
O17			0.109	0.771									1.064	1.94
O18		0.568	0.382	0.278								0.968		2.20
O19		0.091	0.511	0.193									1.056	1.85
	2.09	3.04	2.76	2.98	2.92	3.11	3.19	2.14	4.00	4.07	3.87	3.90	4.02	42.08

Notes: Bond valences are weighted assuming A1 = Ca; A2 = 0.98 Ce + 0.02 Ca; A3 = 0.96 Ce + 0.04 Ca; A4 = 0.95 Ce + 0.05 Ca; M1 = 0.80 Al + 0.20 Mg; M2a = M2b = Al; M3 = 0.35 Fe^{2+} + 0.34 Mg + 0.31 Al; Si1 = Si2 = Si3 = Si4 = Si5 = Si.

similar to the corresponding tetrahedra in epidote; likewise, the Si4 and Si5 tetrahedra can be compared to the tetrahedral sites in törnebohmite (1.632 and 1.619 Å, Shen and Moore 1982). We can therefore reasonably assume that no substitution of Si by other cations occurs at these sites.

Hydrogen bonding

Anions not coordinated to Si are O4 and O10 within the E modules, and O11 within the T modules. As expected on the basis of the close structural relationship between gatelite-(Ce) and the parent minerals, two H atoms were found, at 0.98 Å from O10 and 1.01 Å from O11, respectively. Accordingly, the following O-O contacts suitable for hydrogen bonding (not polyhedral edges) were observed: O10-O15 = 2.655(6) Å and O11-O4 = 2.916(6) Å. An electrostatic charge balance (Table 7) was then computed according to Brese and O'Keeffe (1991). In accord to the predicted model, the bond-valence sums for the involved O atoms are: 1.35 (O10), 1.37 (O11), 1.56 (O15), and 1.67 (O4) v.u. A sum of 1.35–1.37 v.u. is indeed rather high for a hydroxyl oxygen atom, and might indicate partial occupancy of these sites by O^{2-}, as required by the stoichiometry. A refinement of the occupancy of the anion positions (O vs. F) was attempted, and the results suggested possible $F^- \leftrightarrow O^{2-}$ substitution at the O4 site. This is in keeping with what was observed in dollaseite-(Ce), where F^- is completely ordered at this site (Peacor and Dunn 1988).

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