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ALLANITE-(La) FROM BUCA DELLA VENA MINE, APUAN ALPS, ITALY, AN EPIDOTE-GROUP MINERAL

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ABSTRACT

Allanite-(La) is a member of the epidote group. It was sampled at Buca della Vena mine, near Stazzema, Apuan Alps, Tuscany, Italy. It occurs as prismatic crystals up to 2-3 mm in length along [010] within barite veins cutting a dolomitic metamorphosed limestone. The mineral is black with brownish reflections, a brown streak and a vitreous luster, transparent to translucent, nonfluorescent, brittle with a conchoidal fracture. The observed forms are {001}, {100}, {101}, {101}, {210}, {011}, and the cleavage is imperfect along {001}. The hardness (Mohs) is about 6, D(obs.) 3.93(1), D(calc.) 3.94 g/cm³. Optically, allanite-(La) is biaxtal, with $n_x = 1.755(5)$, $n_y = 1.760(5)$, $n_z = 1.765(5)$, $2V = 90(2)^\circ$, very high dispersion and strong pleochroism from greenish to greenish brown. The chemical composition of allanite-(La) has been determined by electron-microprobe analysis and points to $the following empirical formula: Ca_{1.000} \left[(La_{0.288}Ce_{0.206}Nd_{0.116}Pr_{0.106}Y_{0.001})_{\Sigma 0.717}Ca_{0.279}Th_{0.006} \right]_{\Sigma 1.002} (Al_{0.899}Fe^{3+}_{0.101})_{\Sigma 1.000} Al_{1.000} Al_{1.000} Al_{0.001} Al_{0$ $(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Mg_{0.044}Ti_{0.007})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_2O_7) O (OH). The simplified formula is Ca(REE,Ca)Al_2(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Mg_{0.044}Ti_{0.007})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_2O_7) O (OH). The simplified formula is Ca(REE,Ca)Al_2(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Mg_{0.044}Ti_{0.007})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_2O_7) O (OH). The simplified formula is Ca(REE,Ca)Al_2(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Mg_{0.044}Ti_{0.007})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_2O_7) O (OH). The simplified formula is Ca(REE,Ca)Al_2(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Ng_{0.044}Ti_{0.007})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_2O_7) O (OH). The simplified formula is Ca(REE,Ca)Al_2(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Ng_{0.044}Ti_{0.077})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] ($ $Fe^{3+}(SiO_4)(Si_2O_7)O(OH)$ (Z = 2). The six strongest lines in the X-ray powder-diffraction pattern [d in Å(1)(hkl)] are: 3.506(20)(211), 2.901(100)(113), 2.860(40)(020), 2.692(60)(013), 2.611(50)(311), and 2.174(25)(401). Allanite-(La) is monoclinic, $P2_1/m$, with a 8.914(4), b 5.726(1), c 10.132(6) Å, β 114.87(5)°, V 469.1(3) Å³. The crystal structure of allanite-(La) has been refined to R = 0.0328 for 1985 independent reflections collected via single-crystal X-ray-diffraction measurements. The name allanite-(La) recalls the relationship with allanite-(Ce), the Levinson modifier indicating the dominant REE. The root name honors the Scottish mineralogist Thomas Allan (1777-1883). Although the name allanite-(La) has been already used in the literature, the mineral had not been officially approved. The recognition and complete characterization of allanite-(La) from Buca della Vena mine, which now has to be considered the type locality of the mineral, fill a gap in the systematics of the epidote group.

Keywords: allanite-(La), epidote group, lanthanum, new mineral species, Buca della Vena mine, Italy, electron-microprobe data, X-ray powder data, crystal structure.

Sommaire

L'allanite-(La) fait partie du groupe de l'épidote. Nous l'afons échantillonné à la mine de Buca della Vena, près de Stazzema, Alpes Apouennes, en Toscane, Italie. Elle se présente en cristaux prismatiques atteignant une longueur de 2-3 mm selon [010] dans des veines de barite recoupant un calcaire dolomitique métamorphisé. Le minéral est noir avec des réflexions brunâtres, une rayure brune et un éclat vitreux; les cristaux sont transparents à translucides, non-fluorescents, cassants, avec une fracture conchoidale. Nous trouvons les formes $\{001\}$, $\{100\}$, $\{101\}$, $\{10\bar{1}\}$, $\{210\}$, et $\{011\}$, et le clivage est imparfait le long de $\{001\}$. La dureté de Mohs est d'environ 6; la densité observée est 3.93(1), et la densité calculée, 3.94 g/cm³. Optiquement, l'allanite-(La) est biaxe, avec $n_x 1.755(5)$, $n_y 1.760(5)$, $n_z 1.765(5)$, et un 2V de 90(2)°, une très forte dispersion et un pléochroïsme intense allant de vert à brun verdâtre. La composition chimique de l'allanite-(La) a été établie par analyses à la microsonde électronique, et indique la formule empirique Ca_{1.000} [(La_{0.288}Ce_{0.206}Nd_{0.116}Pr_{0.106}Y_{0.001}) $\Sigma_{0.717}$ Ca_{0.279}Th_{0.006}] $\Sigma_{1.002}$ (Al_{0.899}Fe³⁺0.101) $\Sigma_{1.000}$ Al_{1.000} $(Fe^{2+}_{0.669}Fe^{3+}_{0.279}Mg_{0.044}Ti_{0.007})_{\Sigma 0.999} [(Si_{0.978}Al_{0.022})_{\Sigma 1.000}O_4] (Si_2O_7) O (OH). La formule simplifiée serait Ca(TR,Ca)Al_2(Fe^{2+}, Ca)Al_2(Fe^{2+}, Ca)$ Fe^{3+})(SiO₄)(Si₂O₇)O(OH) (Z = 2). Les six raies les plus intenses du spectre de diffraction X (méthode des poudres) [d en Å(I)(hkl)] sont: 3.506(20)(211), 2.901(100)(113), 2.860(40)(020), 2.692(60)(013), 2.611(50)(311) et 2.174(25)(401). L'allanite-(La) est monoclinique, $P2_1/m$, avec a 8.914(4), b 5.726(1), c 10.132(6) Å, β 114.87(5)°, V 469.1(3) Å³. Nous en avons déterminé la structure cristalline jusqu'à un résidu R de 0.0328 en utilisant 1985 réflexions indépendantes prélevées sur monocristal. Le nom rappelle la relation de cette espèce avec l'allanite-(Ce), le suffixe de Levinson indiquant la terre rare dominante. La racine du nom honore le minéralogiste écossais Thomas Allan (1777-1883). Quoique l'allanite-(La) ait déjà été signalée dans la littérature, le nom avait été utilisé sans l'approbation officielle. Son homologation et la caractérisation complète du matériau de la mine Buca della Vena mine, qui devient ipso facto la localité-type de l'espèce, comblent une lacune dans la systématique du groupe de l'épidote.

(Traduit par la Rédaction)

Mots-clés: allanite-(La), groupe de l'épidote, lanthane, nouvelle espèce minérale, mine Buca della Vena, Italie, données de microsonde électronique, spectre de diffraction X sur poudre, structure cristalline.

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INTRODUCTION

The general formula of epidote-group minerals is $A_2M_3(SiO_4)(Si_2O_7)O(OH)$. Monoclinic epidotes, which display a great chemical variability, can be conventionally divided into two subgroups, which are distinguished on the basis of the dominant cation at the A2 site: the allanite subgroup (A2 = REE) and the epidote subgroup $(A2 \neq REE)$. Within the allanite subgroup, different root names denote minerals differing in the dominant atom at one or more of the key sites, namely the three independent octahedral sites M1, M2, and M3, the larger A1 site, and the O4 site, which besides oxygen may be occupied by fluorine (cf. Table 1). As usual, for each given root-name. Levinson modifiers denote minerals that differ only in the rare-earth element that is dominant. According to the guidelines of the IMA Commission on New Minerals and Mineral Names, minerals differing in the dominant REE should be regarded as distinct mineral species, and as such they should be officially approved by the CNMMN.

The root name "allanite", which honors the Scottish mineralogist Thomas Allan (1777-1833), who first studied the mineral, denotes the epidote with the following combination of atoms at the key sites: A1 = Ca, A2 = REE, M1 and $M2 = AI, M3 = Fe^{2+},$ O4 = O. The mineral originally described as allanite from Iglorsoit, Greenland (Thomson 1810) is actually allanite-(Ce), and for reasons of priority, the name allanite-(Ce) was formally approved by CNMMN (Nickel & Mandarino 1987). Although cerium is the dominant REE in most samples of allanite, chemical data are available in the literature for allanite (and for others REE-bearing epidotes as well) which should be given the status of mineral species but were never formally approved, although suitable mineral names have been circulating (Levinson 1966, Bayliss & Levinson 1988). With the aim of defining the status of IMA-approved species for such orphan epidotes, in the context of the revision of the nomenclature of epidote-group minerals

TABLE 1. IMA-APPROVED SPECIES OF THE ALLANITE SUBGROUP OF THE EPIDOTE GROUP

Mineral	Key sites							
	Al	A2	M1	М2	МЗ	04		
Allanite-(Ce)	Са	REE (Ce)	Al	Al	Fe ²⁺	0	(1)	
Dollaseite-(Ce)	Ca	REE (Ce)	Mg	Al	Mg	F	(2)	
Dissakisite-(Ce)	Ca	REE (Ce)	Al	Al	Mg	0	(3)	
Khristovite-(Ce)	Ca	REE (Ce)	Mg	A1	Mn ²⁺	F	(4)	
Androsite-(La)	Mn ²⁺	REE (La)	Mn ³⁴	Al	Mn ²⁺	0	(5)	
Ferriallanite-(Ce)	Ca	REE (Ce)	Fe ³⁺	Al	Fe ²	0	(6)	
Allanite-(La)	Ca	REE (La)	Al	Al	Fe ²	0	(7)	

References: (1) Thomson (1810), (2) Peacor & Dunn (1988), (3) Grew *et al.* (1991), (4) Pautov *et al.* (1993), (5) Bonazzi *et al.* (1996), (6) Kartashov *et al.* (2002), (7) this work.

being carried out by an ad hoc IMA Subcommittee (T. Armbruster, pers. commun.), we describe herewith the new mineral allanite-(La). As already stated, allanite-(La) is not a "new" mineral species in the broad sense: a selection of localities at which compositions of epidotes corresponding to allanite-(La) have been reported is given below. Our objective in this paper is to fill the gap in the mineralogical literature, and to provide an official certificate of birth for allanite-(La). The mineral and its name were approved by the IMA CNMMN (proposal # 2003–065). The name of course reflects the relationships with allanite-(Ce), the Levinson modifier indicating the dominant REE. The type specimen of allanite-(La) is stored at "Centro Interdipartimentale Museo di Storia Naturale e del Territorio" of the University of Pisa, under the catalogue No. 10478.

OCCURRENCE

Allanite-(La) was found at the Buca della Vena mine, near Stazzema (LU), Apuan Alps, Tuscany, Italy. The above locality should be considered from now on the type locality for allanite-(La), with the approval by the CNMMN. The mineral is closely associated with calcite and barite, and occurs within barite veins cutting a dolomitic metamorphic limestone (a geological formation denoted with the Italian term "grezzoni"), in a specific zone of the mine known as "Castello". The Buca della Vena mine is a well-known small mineralized orebody of microcrystalline hematite, magnetite, pyrite, and barite, and it represents the type locality for many other mineralogical species such as apuanite, versiliaite, dessauite, scainiite, pillaite, pellouxite, and rouxelite (Orlandi & Dini 2004).

At this locality, tiny black prismatic crystal of allanite-(Ce) were also found in other quartz veins located in a different part of the Buca della Vena mine; allanite-(Ce) occurs there together with monazite-(Ce), dessauite, pyrite, anatase, gypsum and diadochite.

PHYSICAL PROPERTIES

At the Buca della Vena mine, allanite-(La) occurs as prismatic crystals, elongate along [010], up to 2–3 mm in length. In general, it is well crystallized and definitely non metamict. The observed forms are {001}, {100}, {101}, {101}, {210}, and {011}. Crystals are black with brownish reflections, a brown streak, and a vitreous luster. Allanite-(La) is transparent to translucent and non-fluorescent, brittle with a conchoidal fracture, and shows an imperfect cleavage along {001}. The hardness (Mohs) is *ca*. 6. The density was measured with heavy liquids and is 3.93(1) g/cm³; the calculated value is 3.94 g/cm³.

Opically, allanite-(La) is biaxial, with n_x 1.755(5), n_y 1.760(5), n_z 1.765(5), $2V = 90(2)^\circ$. The dispersion is very high. Orientation: Y = b. The pleochroism is strong, with Y greenish to olive green and $\sim Z$ greenish brown.

CHEMICAL DATA

The chemical analysis of allanite-(La) was carried out with an ARL-SEMQ electron microprobe, and results are reported in Table 2. Operating conditions were: WDS mode, 15 kV, 20 nA, beam diameter 10 μ m. The following standards were used: microcline (Si, Al), ilmenite (Ti, Fe), synthetic ThO₂ (Th), synthetic Chicago glass (Y, La, Ce, Pr, Nd), olivine (Mg), and clinopyroxene (Ca). All other elements with $Z \ge 9$ were below the detection limit. The amount of CO₂ was not measured, as carbonate groups are known to be incompatible with the epidote structure. The amount of H₂O was not measured directly owing to the scarcity of material; it was computed assuming an ideal content of 1 (OH) per formula unit.

The following empirical formula was obtained from the average data, and it was recalculated as to give 8 cations and 12.5 atoms of oxygen on anhydrous basis, namely 12 O + 1 (OH): Ca_{1.000} [(La_{0.288} Ce_{0.206}Nd_{0.116}Pr_{0.106}Y_{0.001}) $\Sigma_{0.717}$ Ca_{0.279}Th_{0.006}] $\Sigma_{1.002}$ (Al_{0.899}Fe³⁺_{0.101}) $\Sigma_{1.000}$ Al_{1.000} (Fe²⁺_{0.669}Fe³⁺_{0.279}Mg_{0.044} Ti_{0.007}) $\Sigma_{0.999}$ [(Si_{0.978}Al_{0.022}) $\Sigma_{1.000}$ O4] (Si₂O7) O (OH).

Among the REE, Pr is rather high and, according to Mannucci *et al.* (1986), it could be somewhat overestimated owing to possible interference with La. However, lacking a well-assessed overlap-correction curve, we did not attempt a correction. The simplified formula (Z =2) is Ca(REE,Ca)Al₂(Fe²⁺,Fe³⁺)(SiO₄)(Si₂O₇)O(OH).

We here comment on the recalculation of the chemical formula. Ercit (2002) listed as many as ten different ways adopted by various authors to recalculate compositions of allanite-subgroup minerals obtained with the electron microprobe, *i.e.*, without any direct evaluation of the H₂O content. After a critical appraisal of all proposed approaches, the following are considered by Ercit (2002) as the most valid from the crystal-chemical point of view: (a') 12.5 O and a total of 8 cations, (a") 12 O + 1 (OH) and a total of 8 cations, (b) 6 (M + T) cations and 12 O + 1 (OH).

TABLE 2. CHEMICAL COMPOSITION OF ALLANITE-(La)

SiO, wt%	32.45	32.02 - 32.82	Nd ₂ O ₃	3.53	3.06 - 3.81
TiO	0.10	0.01 - 0.19	MgO	0.32	0.26 - 0.44
ThO,	0.31	0.00 - 0.69	CaO	13.01	11.60 - 14.33
Al ₂ O ₃	17.77	17.10 - 18.54	FeO (total) *	13.67	13.00 - 14.31
Y ₂ O ₃	0.035	0.00 - 0.09	H ₂ O (calc.)*	* 1.63	
La ₂ O ₃	8.51	6.80 - 10.27			
Ce ₂ O ₃	6.12	5.81 - 6.34	Total ***	101.18	
Pr ₂ O ₃	3.16	2.52 - 3.66			

* Recalculated as FeO 8.72, Fe₂O₃ 5.50% on the basis of stoichiometry (so as to give a total of eight non-H cations and 25 positive charges).

** Corresponding to 1 (OH) per formula unit.

Methods (a') and (a'') are two variants of an equivalent approach, the difference lying only in the possibility to have, in the latter case, an estimate of the H₂O content, assuming an ideal stoichiometry. The fixed number of cations and the charge-balance relationship allow the recalculation of the Fe^{2+}/Fe^{3+} value.

In method (b), it is also possible to recalculate the ratio Fe^{2+}/Fe^{3+} on the basis of charge balance and, moreover, it is possible to have a variable number of total cations, *i.e.*, the possibility of vacancies at the A1 and A2 site is considered. As this latter option is supported by both compositional data (Peterson & MacFarlane 1993) and structure refinements (Sokolova *et al.* 1991) for REE-rich epidotes, Ercit (2002) proposed that method (b) is preferable.

In our case, we recalculated the crystal-chemical formula of allanite-(La) according to method (a"). A look at the resulting chemical formula clearly shows that is has exactly 2 A cations and 6 (M + T) cations, and therefore our formula would have been identical also if we had chosen method (b).

X-RAY-DIFFRACTION STUDY

The X-ray powder pattern of allanite-(La) was recorded with a Gandolfi camera (R = 57.3 mm, CuK α radiation, $\lambda = 1.5418$ Å), and is reported in Table 3. The following unit-cell parameters were refined from the indexed powder-diffraction pattern: *a* 8.875(6), *b* 5.735(2), *c* 10.088(7) Å, β 114.88(4)°.

The single-crystal structural study was carried out using a well-shaped prismatic crystal with dimensions $0.4 \times 0.15 \times 0.15$ mm, mounted on a conventional Ital Structures four-circle diffractometer. The following unit-cell parameters were obtained through least-squares refinement of 20 values of 54 accurately centered reflections (18° < 2 θ < 38°): monoclinic, space group $P2_1/m$, a 8.914(4), b 5.726(1), c 10.132(6) Å, β 114.87(5)°, V 469.1(3) Å³. The fractional coordinates of the wellknown structural model of monoclinic epidotes were assumed as starting set (e.g., Dollase 1971) and refined using the SHELXL set of programs (Sheldrick 1993). The occupancies at the cation sites were set in keeping with the chemical composition of our sample of allanite-(La). Neutral-atom scattering curves were those incorporated in SHELXL. For the REE as a whole, the scattering curve of Ce was chosen, whose atomic number is quite close to the average atomic number (58.04) resulting from the chemical analysis. All atom sites were refined assuming full occupancy. In some cases, two different species were refined at the same site, in agreement with the indication of the chemical data, as follows: Ce versus Ca at the A2 site, Al versus Fe at the M1 site, and Fe versus Mg at the M3 site. We also tried to refine the occupancy at the M2 site, but we soon got clear evidence of full occupancy by Al at that site. The crystal-chemical formula resulting from the structural refinement is $[Ca_{1.00}(REE_{0.69}Ca_{0.31})] [(Al_{0.87}Fe_{0.13})Al_{1.00}]$

^{***} Including H_2O (calc.), and the recalculated FeO and Fe₂O₃ instead of FeO (total). The composition reported is the average result of eight analyses.

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TABLE 3. X-RAY POWDER-DIFFRACTION PATTERN OF ALLANITE-(La)

I	d (meas)	d (calc)	hkl	I	d (meas)	d (calc)	hkl
10	9.06	9.15	001	2	1.684	1.684	313
15	7.93	7.92	T01	5	1.659	1.659	T33
5	5.08	5.07	101			1.659	306
5 5 2 2	4.65	4.66	T10	10	1.649	1.648	225
5	4.53	4.57	002			1.646	4 20
2	3.96	3.96	$\bar{2}02$	20	1.632	1.633	233
	3.75	3.76	T12			1.633	214
20	3.506	3.506	211	5	1.620	1.622	313
3	3.293	3.292	210	10	1.601	1.599	331
1	3.112	3.153	$\overline{2}03$	5	1.580	1.577	115
100	2.901	2.897	T13	5	1.550	1.550	510
40	2.860	2.862	020	2	1.530	1.531	421
1	2,806	2.805	211	3	1.513	1.515	234
60	2.692	2.691	013			1.515	T34
50	2.611	2.608	311	1	1.501	1.501	323
5	2,489	2.489	204	5	1.474	1.475	331
5	2.479	2.481	T22			1.473	016
1	2.439	2.429	310	5	1.461	1.463	334
5	2.423	2.426	022			1.463	304
8	2.401	2.398	313	5	1.451	1.451	205
10	2.318	2.320	222	15	1.432	1.432	613
15	2.283	2.286	T14			1.432	431
5	2.221	2.218	402	3	1,410	1.410	516
25	2.174	2.166	401			1.410	614
10	2.142	2.146	403			1.409	T40
15	2.120	2.119	223	2	1.396	1.398	605
10	2.089	2.087	023			1.397	233
3	2.019	2.016	205	_		1.395	106
3	1.985	1.991	104	5	1.380	1.381	426
_		1.980	404	3	1.362	1.362	241
3	1.942	1.939	305	2	1.351	1.351	502
10	1.902	1.902	222	. 8	1.304	1.304	622
10	1.879	1.879	224	-		1.304	243
3	1.856	1.856	130	5	1,274	1.276	423
		1.855	T31			1.275	531
10	1.778	1.778	405	2	1.263	1.263	704
10	1.755	1.753	422	-		1.263	340
-	1 700	1.753	231	5	1.248	1.247	T27
5	1.729	1.727	421			1.247	208
-		1.727	411	1	1.233	1.233	714
5	1.699	1.704 1.697	$\frac{204}{415}$	1	1.221	1.221	522
		1.697	4 15				

Gandolfi camera, R = 57.3 mm, CuKa, $\lambda = 1.5418$ Å. Intensities were estimated with the help of a digitalized pattern.

 $(Fe_{0.88}Mg_{0.12})]$ (SiO₄) (Si₂O₇) O (OH), which is in fairly good agreement with the formula obtained with EPMA. All atoms were refined anisotropically except hydrogen, which was refined isotropically without any positional constraint. The greatest $r_{\text{max}}/r_{\text{min}}$ value among axes of the thermal ellipsoids is 2.36 for O1. The two highest electron-density peaks in the final difference-Fourier synthesis (3.1 and 2.5 $e/Å^3$) are located in the vicinity of the A2 site, and are likely to represent nothing more than the result of minor experimental flaws. All other positive and negative peaks are less than $1.7 e/Å^3$. Other details of the collection and refinement of intensity data, the final coordinates and displacement parameters of atoms, and the bond distances are given in Tables 4, 5, and 6, respectively. A table of structure factors can be obtained from the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2, Canada.

TABLE 4. SELECTED EXPERIMENTAL DATA FOR THE STRUCTURAL STUDY OF ALLANITE-(La)

Diffractometer	Ital Structures
Radiation, generator setting	MoKα (λ = 0.71069 Å), 50 kV, 30 mA
Unit-cell parameters	a 8.914(4), b 5.726(1), c 10.132(6) Å, B 114.87(5)°
Space group	$P2_{1}/m$
Scan range (indices and 20)	$0 \le h \le 14, -9 \le k \le 9, -16 \le l \le 16, 5^{\circ} \le 20 < 70^{\circ}$
Scan width (in θ)	±0.5°
Scan speed	1 to 8°/min
Absorption correction	y-scan measurements on two reflections
Transmission factor range	0.877 ÷ 1.164
Measured intensities	3854
Independent reflections	2003
R _{ini} from merging equivalents	0.0720
Observed reflections	1985
$[F_{o} > 4\sigma(F_{o})]$	
Max. Δ/σ in the last l.s. cycle	0.001
Refined parameters	124
Final R indices	R1 = 0.0328 (observed reflections),
	0.0336 (all data); wR2 = 0.0944, S = 1.178
Max peak and hole	+3.08 and -1.70 e/Å ³
in the ΔF map	

The main structural features of allanite-(La) are the same as those of many other monoclinic epidotes and will not be discussed in detail. The only result worth pointing out is the good match between structural parameters, in particular the average bond-distances, and the peculiar chemical composition of allanite-(La).

OTHER OCCURRENCES OF ALLANITE-(LA)

As already stated, chemical compositions corresponding to allanite-(La) have already been reported in the literature. Here is a selection of localities at which allanite-(La) has been found: Barringer Hill, Llano County, Texas, USA (Marble 1940), Wilmot Pass, Fiordland, New Zealand (Hutton 1951a), Ragged Peak, Yosemite National Park, Tuolumne County, California, USA (Hutton 1951b), North Karelia, Russia (Zhirov et al. 1961), several localities in Romania (Boul massif, Poiana Ruscă Mountains; Sebeş Valley and Pietrosu Valley, Sebes Mountains; Mîndra Ridge, Parîng Mountains; Lotru valley, Lotru Mountains) (Pavelescu & Pavelescu 1972), Mt. Falconer, Lower Taylor Valley, South Victoria Land, Antarctica (Ghent 1972). A few other occurrences are reported in Deer et al. (1986). At some of the above localities, the occurrence of allanite-(La) instead of allanite-(Ce) seems to be the result of a statistical accident, namely the existence of one or a few compositions with La > Ce among several with Ce >La. At Buca della Vena mine - Castello, the dominance of La over Ce is strong and constant.

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TABLE 5. FINAL FRACTIONAL AND DISPLACEMENT PARAMETERS FOR ALLANITE-(La)

Site	x	У	Ζ	U_{11}	U ₂₂	U_{33}	U_{23}	U_{13}	<i>U</i> ₁₂	U_{eq}
A1	0.7590(1)	3/4	0.15183(9)	0.0161(3)	0.0098(3)	0.0149(3)	0	0.0083(3)	0	0.0130(2)
A2	0.59437(3)	3/4	0.42901(3)	0.0091(1)	0.0125(1)	0.0124(1)	0	0.00294(9)	0	0.01187(9)
M1	0	0	0	0.0070(4)	0.0056(4)	0.0113(4)	-0.0005(3)	0.0030(3)	-0.0001(3)	0.0083(3)
М2	0	0	1/2	0.0067(4)	0.0055(4)	0.0128(5)	-0.0003(4)	0.0033(3)	0.0005(4)	0.0086(2)
М3	0.29816(8)	1/4	0.21552(7)	0.0076(3)	0.0092(3)	0.0129(3)	0	0.0017(2)	0	0.0108(2)
Sil	0.3374(1)	3⁄4	0.0394(1)	0.0077(4)	0.0071(4)	0.0113(4)	0	0.0029(3)	0	0.0091(2)
Si2	0.6852(1)	1/4	0.2793(1)	0.0075(4)	0.0076(4)	0.0115(4)	0	0.0036(3)	0	0.0090(2)
Si3	0.1857(1)	3/4	0.3217(1)	0.0071(4)	0.0078(4)	0.0108(4)	0	0.0036(3)	0	0.0086(2)
01	0.2326(2)	0.9899(4)	0.0302(2)	0.0109(7)	0.0080(8)	0.0225(9)	0.0034(8)	0.0079(7)	0.0014(7)	0.0135(4)
O2	0.3094(2)	0.9736(4)	0.3634(2)	0.0121(7)	0.0135(9)	0.0171(8)	-0.0029(8)	0.0067(6)	-0.0051(8)	0.0140(4)
O3	0.7948(2)	0.0139(4)	0.3403(2)	0.0083(7)	0.0079(8)	0.0155(8)	-0.0018(7)	0.0006(6)	0.0005(7)	0.0121(4)
O4	0.0550(3)	1/4	0.1294(3)	0.009(1)	0.008(1)	0.014(1)	0	0.0034(9)	0	0.0107(5)
05	0.0471(4)	3/4	0.1495(3)	0.011(1)	0.010(1)	0.013(1)	0	0.0042(9)	0	0.0115(5)
06	0.0651(4)	3⁄4	0.4083(3)	0.010(1)	0.007(1)	0.016(1)	0	0.0077(9)	0	0.0106(5)
07	0.5104(4)	3/4	0.1792(3)	0.009(1)	0.015(1)	0.014(1)	0	0.0022(9)	0	0.0138(5)
08	0.5364(4)	1/4	0.3269(4)	0.012(1)	0.025(2)	0.022(1)	0	0.011(1)	0	0.0183(6)
09	0.6165(4)	1/4	0.1017(3)	0.017(1)	0.023(2)	0.014(1)	0	0.006(1)	0	0.0180(6)
010	0.0830(4)	1/4	0.4269(3)	0.010(1)	0.009(1)	0.014(1)	0	0.0053(9)	0	0.0106(5)
H10	0.06(1)	1/4	0.35(1)							0.06(3)

Refined site-occupancies: A2 = 0.689(3) REE (Ce) + 0.311(3) Ca; M1 = 0.871(7) A1 + 0.129(7) Fe; M3 = 0.880(8) Fe + 0.120(8) Mg.

TABLE 6. SELECTED BOND-DISTANCES (Å) FOR ALLANITE-(La)

Al - 07	2.346(3)	MI - O4	1.862(2)	Sil - 07	1.596(3)
A1 - O3	2.349(2)	M1 - O4'	1.862(2)	Si1 - O1	1.642(2)
A1 - O3'	2.349(2)	M1 - O1	1.965(2)	Sil - Ol'	1.642(2)
A1 - O1	2.396(2)	M1 - O1'	1.965(2)	Si1 - O9	1.645(4)
A] - O[`	2.396(2)	M1 - O5	1.997(2)		
A1 - O5	2.579(3)	M1 - O5'	1.997(2)	Average	1.631
Al - O6	2.870(4)				
A1 - O9	3.086(1)	Average	1.941	Si2 - O8	1.591(3)
Al - O9'	3.086(1)	-		Si2 - O3	1.630(2)
A1 - O9''	3.251(4)	M2 - O3	1.865(2)	Si2 - O3'	1.630(2)
		M2 - O3'	1.865(2)	Si2 - O9	1.638(4)
Average	2.671	M2 - O10	1.899(2)		
0		M2 - O10'	1.899(2)	Average	1.622
A2 - O7	2.318(3)	M2 - O6	1.924(2)		
A2 - O2	2.479(2)	M2 - O6'	1.924(2)	Si3 - O2	1.625(2)
A2 - O2'	2.479(2)			Si3 - O2'	1.625(2)
A2 - O10	2.621(3)	Average	1.896	Si3 - O6	1.650(3)
A2 - O2"	2.667(3)			Si3 - O5	1.660(3)
A2 - O2'''	2.667(3)	M3 - O8	1.941(4)		
A2 - O3	2.763(2)	M3 - O4	1.967(3)	Average	1.640
A2 - O3`	2.763(2)	M3 - O2	2.153(3)	-	
A2 - O8	3.014(1)	M3 - O2`	2.153(3)	O10 - H10	0.76(10)
A2 - O8'	3.014(1)	M3 - O1	2.272(3)	O10 O4	2.918(5)
A2 - O8''	3.146(4)	M3 - O1'	2.272(3)		
Average	2.721	Average	2,126		
0					

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