

Lukechangite-(Ce), a new rare-earth-fluorocarbonate mineral from Mont Saint-Hilaire, Quebec

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ABSTRACT

Lukechangite-(Ce), ideally $\text{Na}_3\text{Ce}_2(\text{CO}_3)_4\text{F}$, is a new mineral from Mont Saint-Hilaire, Quebec. It occurs as tabular, short prismatic, and barrel-shaped crystals up to 1 mm. It is colorless to pale beige with a white streak and a vitreous, or somewhat pearly on {0001}, luster. Associated minerals include microcline, analcime, sodalite, aegirine, serandite, eudialyte, catapleite, fluorite, petersenite-(Ce), siderite, astrophyllite, and albite. Lukechangite-(Ce) is soft, Mohs hardness $\approx 4\frac{1}{2}$, brittle, with an uneven to conchoidal fracture, and with perfect {0001} cleavage. Lukechangite-(Ce) is uniaxial negative, $\omega = 1.728(3)$ and $\epsilon = 1.542(1)$. It is hexagonal, space group $P6_3/mmc$, $a = 5.068(1)$, $c = 22.87(5)$ Å, $V = 509(1)$ Å³, and $Z = 2$. The strongest X-ray powder diffraction lines [d (Å), I , hkl] are: 5.71(50)(004), 4.31(100)(101), 3.804(50)(006), 3.169(70)(105), 2.877(60)(106), 2.534(70)(110), 2.192(90B)(109,200,201), 1.978(70)(205), and 1.658(50)(209,210,211). An average of the electron-microprobe analyses gave Na_2O 14.94, CaO 0.10, SrO 0.12, La_2O_3 16.36, Ce_2O_3 29.48, Pr_2O_3 1.95, Nd_2O_3 5.88, F 3.58, CO_2 (28.40), and $\text{O} \equiv \text{F} - 1.51$, total 99.30 wt%. CO_2 was calculated by stoichiometry from the results of the crystal-structure analysis. D_{calc} is 4.02 g/cm³. The atomic arrangement of lukechangite-(Ce) has been refined to $R = 3.4\%$. The structure is layered parallel to (001), with CO_3 groups oriented parallel to the layering forming thick slabs incorporating either Ce or Na cations and a separate Na-F layer. The structure of lukechangite-(Ce) resembles that of huanghoite-(Ce) and baiyuneboite-(Ce) and is isostructural with synthetic $\text{Na}_3\text{La}_2(\text{CO}_3)_4\text{F}$.

INTRODUCTION

There are 34 rare-earth-element (REE) fluorocarbonate mineral species known and these provide the major economic sources of REE. Many of the new REE carbonate minerals being described today will not likely ever be of economic interest because of their existence only in small quantities, but their value may be in their crystal-chemical properties. Recently there has been a great deal of interest in fluorocarbonates for industrial applications, and hence many have been synthesized. REE fluorocarbonates have useful optical properties and the 3d transition-metal fluorocarbonates are being investigated for their magnetic properties. Many of the synthesized compounds have natural equivalents whereas others have not yet been found as minerals. The synthetic equivalents are extremely valuable study material for mineralogists as many of the minerals are not found in crystals suitable for crystal-structure analysis (Mercier and Leblanc 1993a, 1993b, and 1993c). The new mineral lukechangite-(Ce) is another REE-fluorocarbonate mineral that has not been previously reported in nature yet has a synthetic, isostructural phase that was previously characterized.

Mont Saint-Hilaire is known throughout the world for its diversity in mineral species. This diversity results from the complex geochemical history of the locality, of which

lukechangite-(Ce) serves as yet another example. At this locality 41 carbonate minerals have been identified (Horváth and Gault 1990), as well as approximately ten unknowns (Chao et al. 1990). Of the identified carbonates, 17 contain rare earths as essential elements (Grice 1996), and of these six contain fluorine as an essential anion: bastnäsite-(Ce), cordylite-(Ce), horváthite-(Y) (Grice and Chao 1997), parisite-(Ce), reederite-(Y), and synchysite-(Ce).

The new mineral described here, lukechangite-(Ce), found originally in the Poudrette quarry, Mont Saint-Hilaire, Rouville County, Quebec, is named in honor of Luke L.Y. Chang (1934), University of Maryland, for his contributions to the study of carbonate group minerals. The new mineral and the name were approved by the Commission on New Minerals and Mineral Names, IMA. Cotype material is housed in the collection of the Canadian Museum of Nature under catalogue no. CMNMI 81535.

Occurrence

Mont Saint-Hilaire is an alkaline intrusive complex and one of the ten Monteregian Hills, a series of plutons that are aligned along the St. Lawrence Valley for almost 150 km east from Oka to Megantic, Quebec.

TABLE 1. X-ray powder diffraction data for lukechangite-(Ce) and related minerals

Lukechangite-(Ce)*				Baiyuneboite-(Ce)†		Cordylite-(Ce)‡		Huanghoite-(Ce)§	
<i>l</i>	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>hkl</i>	<i>l</i>	<i>d</i> _{obs}	<i>l</i>	<i>d</i> _{obs}	<i>l</i>	<i>d</i> _{obs}
10	11.47	11.43	002			5	11.535		
50	5.71	5.72	004			30	5.766		
100	4.31	4.31	101	50	4.320	80	4.366		
5	4.10	4.10	102	40	4.120	60	4.128		
50	3.804	3.812	006	70	3.840	80	3.843	70	3.91
		3.804	103						
40	3.479	3.482	104	90	3.510	90	3.510		
70	3.169	3.167	105	100	3.200	100	3.193	100	3.21
60	2.877	2.878	106	50	2.895	50	2.899		
10	2.620	2.621	107						
70	2.534	2.534	110	80	2.547	80	2.550	70	2.50
5	2.473	2.474	112						
15	2.395	2.395	108			5	2.414		
20	2.314	2.317	114			5	2.330		
30	2.286	2.287	0.0.10			20	2.306		
		2.199	109			60	2.216		
90B	2.192	2.195	200	30	2.195	60	2.196		
		2.185	201	20	2.165	60	2.167		
20	2.110	2.110	116	30	2.125	70	2.122		
						30	2.061		
10	2.051	2.049	204	60	2.047	80	2.040	90	2.01
70	1.978	1.979	205	30	1.984	60	1.989		
						10	1.921	100	1.937
40	1.901	1.902	206	40	1.904	60	1.907		
		1.896	118			5	1.891		
20	1.879	1.879	1.0.11			5	1.832		
						10	1.760	40	1.759
30	1.699	1.698	1.1.10			10	1.707		
		1.661	209			10	1.667		
50	1.658	1.659	210						
		1.655	211	10	1.650	10	1.648		
20	1.634	1.633	1.0.13				1.630		
5	1.621	1.621	213			20	1.604	70	1.616
5	1.592	1.593	214	10	1.601	10	1.592		
20	1.559	1.560	215	20	1.564	30	1.569	70	1.557
5	1.530	1.531	1.0.14			10	1.535		
5	1.510	1.509	2.0.11	10	1.480	5	1.518		
10	1.464	1.463	300			20	1.472		
10	1.441	1.440	1.0.15			20	1.451		
5	1.418	1.418	304			20	1.398		
10	1.388	1.389	219			20	1.382		
						10	1.371		
						20	1.351	70	1.335
						10	1.306	60	1.325
								50	1.252
								30	1.201
								50	1.176
								30	1.157
								60	1.083

* Sample from Mont Saint-Hilaire, Quebec, Canada (this study); 114.6 mm Gandolfi camera, CuK α radiation, visual intensities.

† Sample from Baiyunebo, Inner Mongolia, China (Fu and Su 1987).

‡ Sample from Mont Saint-Hilaire, Quebec, Canada (Chen and Chao 1975).

§ Sample from Khibina, Russia (Semenov and Chang 1961).

The cotype specimen was collected in 1995 by Steve and Janet Cares and recognized by G.Y.C as a new species. At present lukechangite-(Ce) must be considered a very rare mineral as there are only a few milligrams known to exist. The specimens were collected in the Poudrette quarry from a large pegmatite dike in the nepheline syenite intrusion. Lukechangite-(Ce) is associated with microcline, analcime, sodalite, aegirine, sérandite, eudialyte, catapleite, fluorite, petersenite-(Ce), siderite, astrophyllite, and albite. Horváthite-(Y) (Grice and Chao 1997), UK96, and UK93 (Chao et al. 1990) were found in a different section of the same pegmatite. This mineral assemblage is thought to be a late-stage pegmatite.

Lukechangite-(Ce) occurs in a late-stage pegmatitic portion of an alkaline, highly agpaite rock. This stage of crystallization favors the presence of cations having weak acid strengths (i.e., cations with a low valence or a large coordination number such as Na and REE). During crystallization weak Lewis acids are stabilized by weak Lewis bases such as F⁻ and (CO₃)²⁻. Hence there is a concentration of REE fluorocarbonates, such as lukechangite-(Ce), in this type of occurrence.

Physical and optical properties

Lukechangite-(Ce) has two distinct habits: (1) tabular, measuring 0.5 to 1.0 mm and (2) short prismatic to barrel-

TABLE 2. Crystallographic and physical properties of lukechangite-(Ce) and related minerals

	Lukechangite-(Ce)*	Baiyuneboite-(Ce)†	Cordylite-(Ce)‡	Huanghoite-(Ce)§
Formula	Na ₃ Ce ₂ (CO ₃) ₄ F	NaBaCe ₂ (CO ₃) ₄ F	BaCe ₂ (CO ₃) ₆ F ₂	BaCe(CO ₃) ₂ F
Symmetry	<i>P6₃/mmc</i>	<i>P6₃/mmc</i>	<i>P6₃/mmc, P62c</i>	<i>R3m</i>
<i>a</i> (Å)	5.061	5.08	5.098	5.072
<i>c</i> (Å)	22.820	23.35	23.050	38.46
<i>Z</i>	2	2	2	6
ω	1.728	1.745	1.773	1.770
ϵ	1.542	1.599	1.576	1.610
<i>D</i> _{calc.} (g/cm ³)	4.02	4.45	3.97	4.84

* Sample from Mont Saint-Hilaire, Quebec, Canada (this study).

† Sample from Baiyunebo, Inner Mongolia, China (Fu and Su 1987).

‡ Sample from Mont Saint-Hilaire, Quebec, Canada (Chen and Chao 1975).

§ Sample from Khibina, Russia (Yang and Pertlik 1993).

shaped crystals, 0.5 to 1.0 mm across. Forms include {0001}, {11 $\bar{2}$ 0}, and {11 $\bar{2}$ 1}, plus at least one more bipyramid. Striations parallel to {0001} are present due to oscillatory growth of the bipyramid. The mineral is colorless to pale beige with a white streak and a vitreous, somewhat pearly on {0001}, luster. It is soft, Mohs hardness \approx 4 $\frac{1}{2}$, brittle, with an uneven to conchoidal fracture and with perfect {0001} cleavage. It does not fluoresce. The mineral sinks readily in methylene iodide (i.e., density > 3.3 g/cm³) and has a calculated density of 4.02 g/cm³. Lukechangite-(Ce) is soluble in 1:1 HCl with effervescence.

Lukechangite-(Ce) is uniaxial negative, $\omega = 1.728(3)$ and $\epsilon = 1.542(1)$ ($\lambda = 589$ nm). A Gladstone-Dale calculation gives a compatibility index of 0.004, which is regarded as superior (Mandarino 1981).

Chemical composition

Chemical analyses were performed on a Cambridge Microscan MK5 electron microprobe. The wavelength-dispersion mode was used with an operating voltage of 15 kV, and the beam current was 0.30 μ A. Data reduction was performed using a modified version of EMPADR VII (Rucklidge and Gasparrini 1969). Five analyses were performed on a single grain using a 50 μ m beam diameter. Data for all elements in the samples were collected for 5 s. Standards used in the probe analyses were: albite (NaK α), hornblende (CaK α), celestine (SrL α), LaAlO₃

(LaL α), CeO₃ (CeL α), PrF₃ (PrL α), NdAlO₃ (NdL α), and LiF (FK α). An average of five electron-microprobe analyses gave Na₂O 14.94, CaO 0.10, SrO 0.12, La₂O₃ 16.36, Ce₂O₃ 29.48, Pr₂O₃ 1.95, Nd₂O₃ 5.88, F 3.58, CO₂ (28.40), and O \equiv F - 1.51, total 99.30 wt%. CO₂ was calculated by stoichiometry from the results of the crystal-structure analysis. The empirical formula based on 12 O atoms is: (Na_{2.99}Ca_{0.01}Sr_{0.01}) $\Sigma_{3.01}$ (Ce_{1.11}La_{0.62}Nd_{0.22}Pr_{0.07}) $\Sigma_{2.02}$ (CO₃)₄F_{1.17} or, ideally, Na₃Ce₂(CO₃)₄F.

X-ray crystallography and crystal structure determination

Precession camera photographs show lukechangite-(Ce) to be hexagonal, diffraction symmetry *6/mmm*, with possible space-group choices *P6₃/mmc* (no. 194), *P6 $\bar{2}$ c* (no. 190), or *P6₃mc* (no. 186) on the basis of systematic absences of reflections. X-ray powder-diffraction data, obtained with a Gandolfi camera are given in Table 1.

Similarities in X-ray powder diffraction patterns (Table 1) and other properties (Table 2) suggest that lukechangite-(Ce) is related to baiyuneboite-(Ce), NaBaCe₂(CO₃)₄F; cordylite-(Ce), BaCe₂(CO₃)₆F₂; and Huanghoite-(Ce), BaCe(CO₃)₂F. Cordylite was originally described from Narssarsuk, Greenland, by Flink (1901). However, a recent study on cordylite-(Ce) (Shen and Mi 1992) showed that an essential amount of Na₂O is present in cordylite-(Ce) from the type locality and the *c* parameter of the mineral calculated from the composition is much smaller than the values observed by Donnay and Donnay (1955) and Chen and Chao (1975). Unpublished microprobe analyses (R.A. Gault, personal communication) confirmed the presence of Na₂O in cordylite-(Ce) from the type locality (3.83 wt%) and from Mont Saint-Hilaire, Quebec (4.01–4.25 wt%). Thus, cordylite-(Ce) is probably identical with baiyuneboite-(Ce).

For the intensity-data measurements a crystal fragment of cotype lukechangite-(Ce) was used. Information relevant to the data collection and structure determination is given in Table 3. Reduction of the intensity data, structure determination, and structure refinement were accomplished by means of the SHELXTL package of computer programs (Sheldrick 1990).

The phasing of a set of normalized structure factors

TABLE 3. Data collection information for lukechangite-(Ce)

Space group	<i>P6₃/mmc</i>
<i>a</i> (Å)	5.0612(8)
<i>c</i> (Å)	22.820(9)
<i>V</i> (Å ³)	506.2(2)
Unit-cell contents 2[Na₃Ce₂(CO₃)₄F]	
Radiation	MoK α
Monochromator	Graphite
μ (mm ⁻¹)	9.10
Measured reflections	1549
Merged reflections	338
Observed reflections (>5 σ_r)	335
Minimum transmission	0.076
Maximum transmission	0.243
Refined parameters	32
<i>R</i> (%)	3.4

TABLE 4. Atomic coordinates, isotropic displacement factors ($\text{\AA}^2 \times 10^3$), and bond-valence sums (v.u.)

Atom	x	y	z	U_{eq}	BVS*
Na1	$\frac{1}{2}$	$\frac{2}{3}$	0.4777(2)	26(1)	0.93
Na2	0	0	$\frac{1}{4}$	21(2)	1.44
Ce	$\frac{2}{3}$	$\frac{1}{3}$	0.35447(2)	7.9(3)	3.16
C1	0	0	0.4358(4)	12(2)	4.15
C2	$\frac{1}{3}$	$\frac{2}{3}$	0.3239(4)	9(2)	4.02
O1	2y	0.1448(6)	0.4375(2)	42(2)	2.07
O2	0.1870(5)	2x	0.3241(2)	16(1)	2.11
F	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	22(3)	0.88

* Constants from Brese and O'Keeffe (1991).

gives a mean value $|E^2 - 1|$ of 0.921, indicative of a centrosymmetric space group. The phased-normalized structure factors, with a combined figure of merit (CFOM) of 0.008, were used to give an E map, which located the Ce, and six lighter element sites. This initial model for least squares refined to $R = 20\%$. The next stages in the structure determination of lukechangite-(Ce) involved establishing the two Na sites, the two CO_3 groups, and the F site. In the final least-squares refinement, all atomic positions were refined with anisotropic displacement factors to a final residual of $R = 3.4\%$. Bond-valence sum calculations (Brese and O'Keeffe 1991) helped to establish the F site.

Table 4 contains the final positional and equivalent isotropic displacement parameters and bond-valence sums, Table 5 contains the selected interatomic distances, Table 6¹ contains anisotropic displacement factors, and Table 7¹ contains observed and calculated structure factors.

Description and discussion of the structure

Lukechangite-(Ce) has three large cation sites, each of which has a distinct coordination polyhedron. Both Na polyhedra have ninefold coordination. The Na1-O₉ polyhedron may be described as a truncated hexagonal pyramid with the corners of the hexagonal base defined by six O1 atoms in a plane just below the Na1 atom and the upper truncation defined by three O1 atoms centered on three of the pyramid faces. The Na2- ϕ_9 polyhedron (ϕ is an unspecified anion) is a regular trigonal prism with three F atoms defining the edges of the equatorial plane and three O1 atoms above and below centering the faces of the prism. The Ce- ϕ_{10} polyhedron is a monocapped

¹ For a copy of Tables 6 and 7, Document AM-97-650, 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 (see inside back cover of a current issue for web address).

hexagonal dipyrmaid with the nine O atoms taking almost the exact positions of the nine O atoms in the Na1- ϕ_9 polyhedron, thus defining the truncated end of the dipyrmaid and the F atom as the apex of the opposite end of the dipyrmaid.

The crystal structure of lukechangite-(Ce) is layered parallel to (001) (Fig. 1a). The layering of REE carbonate minerals was described and depicted in detail by Grice et al. (1994). In lukechangite-(Ce) there are three layers of differing composition: (1) $\text{Na}_2(\text{CO}_3)$, (2) NaF, and (3) $\text{Ce}(\text{CO}_3)$. The carbonate groups are the "flat-lying" type (Grice et al. 1994).

Most REE-fluorocarbonate minerals are layered with "standing-on-edge" CO_3 groups. Of these there are two distinct types (Grice et al. 1997). The members of the bastnäsité-parisite-röntgenite-synchysite group are syntactical intergrowths of various combinations of stacked layers of rare-earth elements, fluorine, alkaline earths, and carbonate groups. The bastnäsité-(Ce) structure (Ni et al. 1993) is an example of this structure type with two types of layer: a CeF layer and a segregated "standing-on-edge" CO_3 layer. Similar syntactical intergrowths are evident in the barium fluorocarbonates cebaite-(Ce) and synthetic $\text{Ba}_2\text{Ce}(\text{CO}_3)\text{F}$ (Mercier and Leblanc 1993a, 1993b), which is likely the newly described mineral 95-040 (Mandarino and Grice 1996) and is either identical to or a polymorph of zhonghaucerite-(Ce). The structure of cebaite-(Ce) (Yang 1995) is an example of mixed layers of "standing-on-edge" CO_3 group sharing the slab with the larger Ba, Ce, and F atoms. The structures of bastnäsité-(Ce) and cebaite-(Ce) are depicted in Grice et al. (1997).

REE fluorocarbonates with crystal structures having "flat-lying" CO_3 groups, as seen in lukechangite-(Ce), are less common than the "standing-on-edge" CO_3 groups described above. Examples of this type of structure are huanghoite-(Ce) (Yang and Pertlik 1993), baiyuneboite-(Ce) [$\text{NaBaCe}_2(\text{CO}_3)_4\text{F}$] (Fu et al. 1987), unnamed mineral $(\text{Ca}_{0.5}\square_{0.5})\text{BaCe}_2(\text{CO}_3)_4\text{F}$ (Shen and Mi 1992), and horváthite-(Y) (Grice and Chao 1997). In contrast to horváthite-(Y) (depicted in Grice and Chao 1997), each of the other minerals has CO_3 layers separate from the layers of F, REE, and alkali or alkaline earths. Baiyuneboite-(Ce) is isostructural with unnamed $(\text{Ca}_{0.5}\square_{0.5})\text{BaCe}_2(\text{CO}_3)_4\text{F}$, lukechangite-(Ce) is isostructural with synthetic $\text{Na}_3\text{La}_2(\text{CO}_3)_4\text{F}$ (Mercier 1994), and huanghoite-(Ce) is isostructural with synthetic $\text{BaSm}(\text{CO}_3)_2\text{F}$ (Mercier and Leblanc 1993a). These three structures differ only slightly within the layering schemes (Fig. 1). The three layers of differing composition may be compared

TABLE 5. Interatomic distances (\AA) for lukechangite-(Ce)

Na1 polyhedron		Na2 polyhedron		Ce polyhedron		C1 triangle		C2 triangle	
Na1-O1	$2.544(7) \times 3$	Na2-O2	$2.356(4) \times 6$	Ce-O1	$2.515(6) \times 3$	C1-O1	$1.270(9) \times 3$	C2-O2	$1.282(4) \times 3$
Na1-O1	$2.698(3) \times 6$	Na2-F	$2.922(1) \times 3$	Ce-O2	$2.630(5) \times 6$				
$\langle \text{Na1-O} \rangle$	2.647	$\langle \text{Na2-}\phi \rangle$	2.545	Ce-F	2.384(1)				
				$\langle \text{Ce-}\phi \rangle$	2.571				

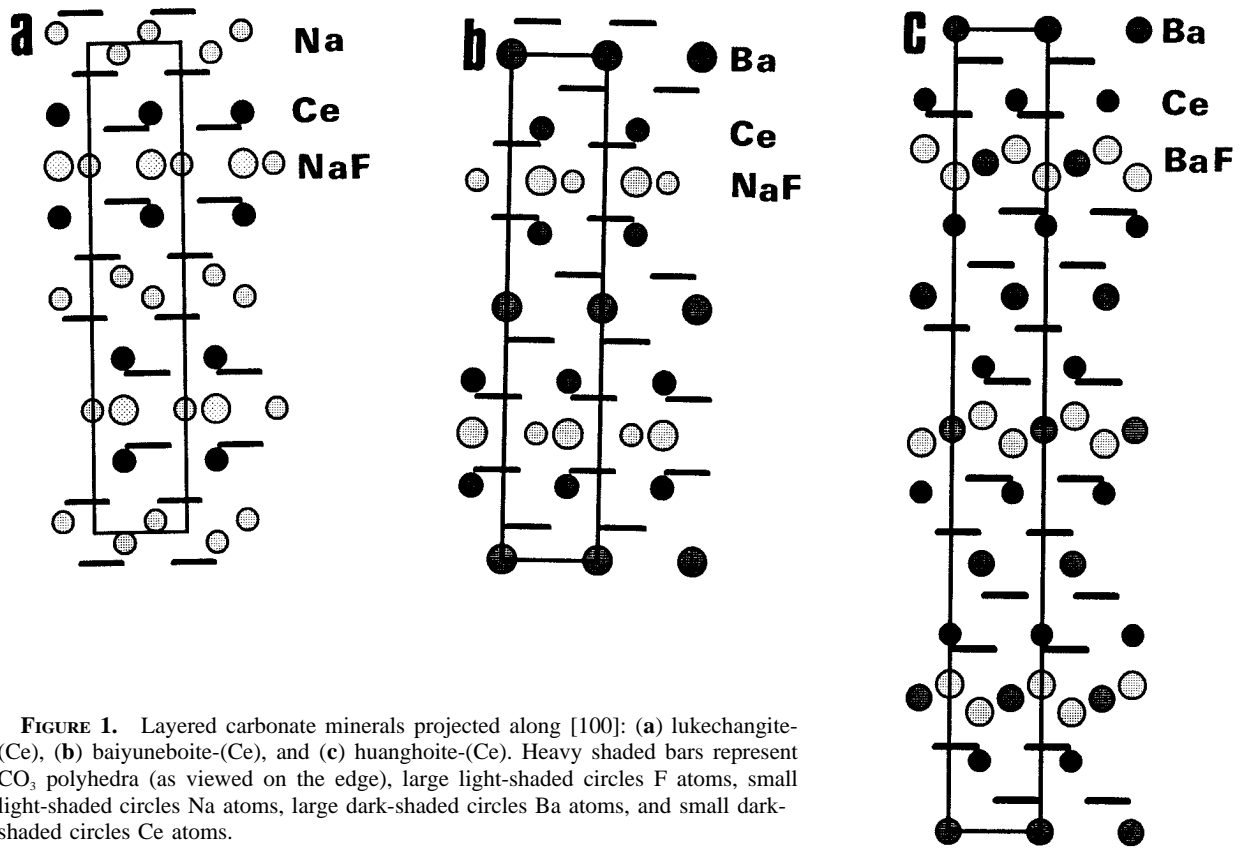


FIGURE 1. Layered carbonate minerals projected along [100]: (a) lukechangite-(Ce), (b) baiyuneboite-(Ce), and (c) huanghoite-(Ce). Heavy shaded bars represent CO_3 polyhedra (as viewed on the edge), large light-shaded circles F atoms, small light-shaded circles Na atoms, large dark-shaded circles Ba atoms, and small dark-shaded circles Ce atoms.

for each structure: lukechangite-(Ce) with (1) $\text{Na}_2(\text{CO}_3)$, (2) $\text{Ce}(\text{CO}_3)_{1.5}$, and (3) NaF; baiyuneboite-(Ce) with (1) $\text{Ba}(\text{CO}_3)$, (2) $\text{Ce}(\text{CO}_3)_{1.5}$, and (3) NaF; and huanghoite-(Ce) with (1) $\text{Ba}(\text{CO}_3)$, (2) $\text{Ce}(\text{CO}_3)_{1.5}$, and (3) BaF_2 . The c cell parameter in each of the “flat-lying” CaCO_3 structures is related to that of a basic slab of $\text{Ca}(\text{CO}_3)$, i.e., multiples of ~ 2.85 Å. For example, aragonite has two slabs ($c = 5.72$ Å), calcite six slabs ($c = 17.06$ Å), lukechangite-(Ce) eight slabs ($c = 22.82$ Å), baiyuneboite-(Ce) eight slabs ($c = 23.17$ Å), and huanghoite-(Ce) twelve slabs ($c = 38.46$ Å) (Table 2). The huanghoite-(Ce)

c cell parameter is somewhat larger than expected due to the added thickness of the BaF_2 layer.

In carbonate minerals with “flat-lying” CO_3 groups there are two basic arrangements, calcite and aragonite (Fig. 2). The aragonite structure in Figure 2 has been referred to a pseudo-hexagonal cell for direct comparison with calcite. Note that the attitude of the CO_3 group in each structure differs by a rotation of 30° with respect to the crystallographic axes. In Figure 2 potential cation sites on the threefold axes, or pseudo-threefold axes, are labeled A and B. In calcite these sites are symmetrically equivalent, with sixfold coordination (Reeder 1983). In aragonite site A has no cation, whereas site B is a ninefold-coordinated site (Speer 1983). It can be readily seen in Figure 3 that lukechangite-(Ce), baiyuneboite-(Ce), and huanghoite-(Ce) all have the orientation of the CO_3 groups in aragonite, not calcite. At first glance the (001) projection of lukechangite-(Ce) resembles that of baiyuneboite-(Ce), and they both differ from huanghoite-(Ce). Closer inspection shows that the arrangement of CO_3 groups around the B site in lukechangite-(Ce) differs by a rotation of 60° from that around the B site of baiyuneboite-(Ce). This difference in orientation of the CO_3 groups has the effect of changing the coordination number for the A site from nine in lukechangite-(Ce) to twelve in baiyuneboite-(Ce). The B site coordination is the same for both minerals; i.e., ninefold if only the li-

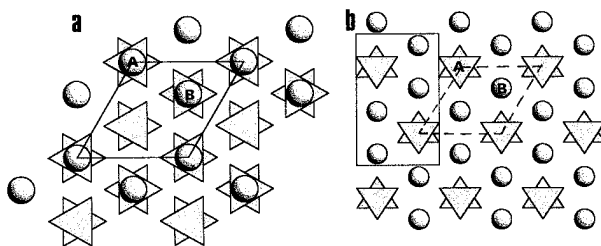


FIGURE 2. The two basic layered structures projected along [001]: (a) calcite and (b) aragonite. Shaded triangles represent CO_3 polyhedra and large dark-shaded circles Ca atoms. The cell for aragonite is outlined with a dashed line. The two types of cation sites available in layered carbonate structures are labeled A and B.

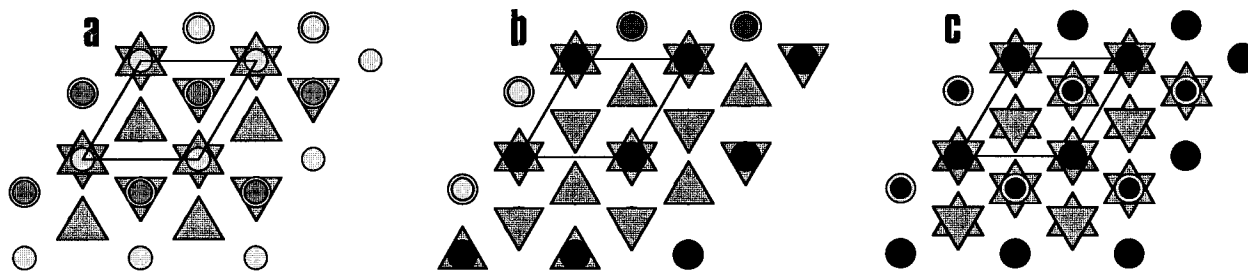


FIGURE 3. Layered structures projected along [001]: (a) lukechangite-(Ce), (b) baiyuneboite-(Ce), and (c) huanghoite-(Ce). Shaded triangles represent CO_3 polyhedra, large light-shaded circles F atoms, small light-shaded circles Na atoms, large dark-shaded circles Ba atoms, and small dark-shaded circles Ce atoms.

gands to O atoms are considered but tenfold if the F atom is added. In huanghoite-(Ce) the A site has 12-fold coordination whereas the B site is 12-fold and tenfold coordinated. Thus the arrangements of CO_3 groups in lukechangite-(Ce), baiyuneboite-(Ce), and huanghoite-(Ce) reveal the mechanism by which each of these structures is able to adapt to size changes in available cations.

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