

LOKKAITE, A NEW HYDROUS RE-CARBONATE FROM PYÖRÖNMAA PEGMATITE IN KANGASALA, SW-FINLAND

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Lokkaite is a new RE-carbonate found in an old pegmatite quarry as a supergene mineral associated with tenerite. Electron microprobe analysis gave: Y-earths 48.7 %, Ce-earths 4.3 %, CaO 3.2 % and Fe₂O₃ 0.4 %. Thermal decomposition gave: CO₂ 32.4 %, H₂O+ 1.6 % and H₂O— 5.4 %, total 96.0 %. When omitting Fe the analysis gives the formula Ca_{0.23}RE_{1.58}(CO_{2.87})₃·1.58 H₂O.

Lokkaite is orthorhombic, the diffraction symbol is *mmmB* - - -; $a_0 = 39.07$ Å, $b_0 = 6.079$ Å and $c_0 = 9.19$ Å. The mineral has a distinct superstructure. The dimensions of the sub-cell are: $a'_0 = \frac{1}{2}a_0$, $b'_0 = b_0$ and $c'_0 = \frac{1}{2}c_0$, and the diffraction symbol is *mmmPb* - -. The strongest X-ray powder lines of lokkaite are: 19.59 (35), 9.77 (50), 6.509 (55), 5.792 (45), 4.594 (75), 3.902 (60), 3.808 (100), 2.931 (40), 2.535 (35) and 2.045 (35).

The colour is white, $\alpha = 1.569$, $\beta = 1.592$ and $\gamma = 1.620$. Elongation is positive and $c \parallel Z$.

The name lokkaite is in honour of the late Professor Lauri Lokka, former Chief Chemist of the Geological Survey of Finland, in recognition of his valuable contributions to the chemistry and mineralogy of the RE-pegmatites of Finland. The name was approved in advance of publication by the Commission on New Minerals and Mineral Names of the IMA.

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Introduction

The supergene carbonate mineralization of the Pyörönmaa pegmatite was detected during the study on the RE-minerals of the pegmatite published by Vormaa *et al.* (1966). In that paper the chemical analysis and the X-ray powder pattern of a hydrous RE-carbonate were given. The mineral was provisionally named tenerite. Later one of the cited authors (A. Vormaa) was

informed by Dr. Akira Kato of the X-ray powder data of tenerite from Iisaka, Japan. Dr. Kato also suggested that the carbonate mineral of Pyörönmaa is not tenerite. At that point the present author received the material of the Pyörönmaa pegmatite for further study.

Occurrence

The main minerals in the Pyörönmaa pegmatite are potash feldspar, albite and quartz;



Fig. 1. Lokkaite incrustations as white radial aggregates on albite. Pyörönmaa, Kangasala. Magn. 8.5 x. Photo: Erkki Halme (in Vormaa *et al.* 1966, Fig. 13).

biotite and garnet occur as minor constituents. The pegmatite is known for its many RE-minerals, such as allanite, gadolinite, britholite, thalenite, fergusonite, bastnäsite and synchysite (Vormaa *et al.*, 1966).

The supergene alteration of the primary minerals of the pegmatite has created new carbonate minerals. The mineral provisionally named tenerite proved to be a new species. It occurs as isolated white radial disc-like aggregates 0.5–1.0 mm in diameter on the surfaces and in the fissures of albite (Fig. 1). In addition to spheroids the mineral occurs as white powdery incrustations intimately associated with tenerite.

The aim of this paper is to give a mineralogical description of the new mineral which is named lokkaite in honour of the late Professor Lauri Lokka, former Chief Chemist of the Geological Survey of Finland. The name lokkaite was

TABLE 1
The chemical composition of lokkaite from Pyörönmaa.

1	2	3
CaO	2.6— 3.4	3.2
Fe ₂ O ₃	0.3— 0.4	0.4
Y ₂ O ₃	29 —29.5	29.0
La ₂ O ₃	0.2— 0.3	0.2
Ce ₂ O ₃	0.6— 1.1	0.7
Pr ₂ O ₃	0.2— 0.4	0.3
Nd ₂ O ₃	1.1— 1.8	1.3
Sm ₂ O ₃	1.6— 2.2	1.8
Gd ₂ O ₃	4.1— 5.4	4.6
Tb ₂ O ₃	1.1— 1.5	1.2
Dy ₂ O ₃	6.2— 8.8	6.8
Ho ₂ O ₃		trace
Er ₂ O ₃	3.1— 4.4	4.0
Tm ₂ O ₃	0.7— 1.2	0.9
Yb ₂ O ₃	1.8— 3.0	2.2
Lu ₂ O ₃		trace
CO ₂		32.4
H ₂ O—		5.4
H ₂ O+		1.6
		96.0

1. Oxide
2. Range of results in per cents
3. Mean value published in Vormaa *et al.*, 1966

Number of microprobe analyses: Ca—Y = 3; La—Lu = 6.

F, Be, Al, Pb, Ti, Mn, Mg, Eu and Si were not detected. Be by optical spectrograph, F by titration, others by microprobe.

approved by the Commission on New Minerals and Mineral Names of the IMA.

Chemistry

The chemical analysis of lokkaite (Table 1) was published by Vormaa *et al.* (1966). Cations were analyzed by an electron microprobe analyzer model »Geoscan» (Be by optical spectrograph). CO₂, H₂O and F were determined by conventional procedures. The amount of pure material available was too small for wet chemical analysis. The samples, total 7.2 mg, from which CO₂ and H₂O were determined were slightly contaminated by tenerite. The analysis suggests the chemical formula Ca_{0.23}RE_{1.58}(CO_{2.87})₃·1.58 H₂O for lokkaite.

X-ray crystallography

Lokkaite was investigated by X-ray powder and single-crystal methods. The crystals are

fibrous and even the smallest fibres used in the single-crystal study were actually crystal bundles. The c -axis of each individual crystal is parallel to the fibre. The reflections on the Weissenberg photographs appear as 1–2 mm long lines.

The approximate unit cell dimensions were measured from the c -axis oscillation and zero-level Weissenberg photographs. More precise dimensions were calculated from the indexed X-ray powder diffraction pattern (Table 2) calibrated by quartz. The unit cell dimensions of lokkaite are:

$$a_0 = 39.07 \text{ \AA}$$

$$b_0 = 6.079 \text{ \AA}$$

$$c_0 = 9.19 \text{ \AA}$$

The intensities of the reflections were measured from the heights of the peaks on the chart. The sample for X-ray spectrometer runs was contaminated by tenerite and albite. The presence of tenerite as an impurity enhances the intensity of reflections 4.596 Å (002) and 2.535 Å (022) of lokkaite and thus the actual intensity of these reflections is smaller than given in Table 2. In any case, the 022-reflection is present on the c -axis second-level Weissenberg photograph and the presence of the 002-reflection was checked by the precession method.

According to the c -axis oscillation and 0-, 1st-, 2nd-, 3rd- and 4th-level Weissenberg photographs the Laue-class of lokkaite is mmm . Only the reflections with $b + l = 2n$ exist, so the possible space groups are: $B222$ (21), $Bm2m$ (35), $Bmmm$ (65) and $B2mm$ (38). The figures in parentheses correspond to the space group numbers in »International tables for X-ray crystallography» (1952). Lokkaite has a distinct superstructure. The dimensions of the sub-cell are: $a'_0 = \frac{1}{2}a_0$, $b'_0 = b_0$ and $c'_0 = \frac{1}{2}c_0$ and the possible space groups $Pb2m$ (26), $Pbm2$ (28) and $Pbmm$ (51).

Physical properties

The crystals of lokkaite in the radial aggregates are straight, brittle fibres. The grain size in the

powdery incrustations of lokkaite and tenerite is less than 0.01 mm and individual crystals cannot be distinguished. The colour is white, sometimes stained to yellow.

The indices of refraction of lokkaite are (Na, 22°C): $\alpha = 1.569$, $\beta = 1.592$ and $\gamma = 1.620$. The crystals are too small for $2V$ measurements by Universal stage. The elongation is positive and $c \parallel Z$.

TABLE 2
X-ray powder data of lokkaite (CuK α , $\lambda = 1.5418 \text{ \AA}$)

hkl	$d(\text{\AA})$	I_{obs}	$\sin^2\theta_{obs}$	$\sin^2\theta_{calc}$
200	19.59	35	0.00155	0.00156
400	9.77	50	.00623	.00623
600*	6.509	55	.01403	.01402
210*	5.792	45	.01771	.01764
410	5.17	5	.02223	.02232
002*	4.594	75 ¹⁾	.02816	.02815
610	4.43	10	.03027	.03010
1000*	3.902	60	.03903	.03893
810*	3.808	100	.04098	.04100
212	3.600	20	.04586	.04580
412	3.427	5	.05060	.05046
020	3.036	5	.06448	.06433
1002	2.978	30	.06701	.06708
812	2.931	40	.06917	.06915
022*	2.535	35 ¹⁾	.09248	.09248
1600	2.443	15	.09957	.09966
1602	2.158	15	.12761	.12781
1810*	2.045	35	.14210	.14222
1620	1.904	10	.16393	.16399
830	1.870	15	.16993	.16965
+ additional lines				

The reflections marked by asterisk (*) were used to calculate the unit cell dimensions

¹⁾ The actual intensity slightly smaller due to the overlapping with tenerite reflections

TABLE 3
Optical properties of lokkaite and related minerals

α	β	γ	
1.569	1.592	1.620	Lokkaite (this paper)
1.555	1.57	1.585	Tengerite, Ytterby, Sweden (Larsen and Berman, 1934)
—	1.56	—	Tengerite, Madagascar (Behier, 1960)
1.622	—	1.642	Tengerite, Iisaka, Japan (Iimori, 1938)
1.611	—	1.636	Tengerite, Kazakhstan (Stepanov, 1961)
1.620	—	1.642	Tengerite, Kazakhstan (Stepanov, 1961)
1.64	—	1.66	Unidentified, Transvaal (Verwoerd, 1963)

TABLE 4
X-ray powder patterns of tenerite and synthetic Y-carbonate

1.		2.		3.		4.		5.		6.	
<i>d</i> (Å)	<i>I</i>	<i>d</i> (Å)	<i>I</i>	<i>d</i> (Å)	<i>I</i>	<i>d</i> (Å)	<i>I</i>	<i>d</i> (Å)	<i>I</i>	<i>d</i> (Å)	<i>I</i>
7.60	m	7.60	m	7.54	60	7.62	80	7.60	90	7.56	60
5.70	m	5.71	s	5.60	60	6.19	20			5.64	85
4.59	s	4.58	s	4.55	70	5.64	50	5.67	70	5.64	85
						5.52	10			4.578	100
						4.60	50	4.59	100		
						4.44	10				
						4.28	10				
		4.12	w								
3.86	s	3.877	s	3.86	100	3.90	100	3.89	70	3.874	75
				3.77	20	3.80	20	3.78	30	3.770	25
3.56	m	3.573	m	3.55	60	3.57	40	3.57	50	3.557	60
						3.52	10				
								3.04	5	3.038	5
2.960	s	2.947	s	2.95	70	2.97	40	2.97	40	2.956	50
						2.92	10	2.92	8	2.921	10
						2.74	30	2.81	3		
2.680	m	2.684	m	2.68	20	2.69	20	2.69	15	2.687	20
						2.64	30				
				2.59	10			2.60	10	2.592	10
2.588	w			2.53	50	2.53	30	2.53	30	2.529	40
2.53	m	2.528	s			2.38	10	2.40	10	2.398	15
		2.392	w			2.37	10	2.37	10	2.365	15
								2.33	5	2.327	5
2.293	w	2.288	w	2.29	30	2.30	10	2.29	10	2.290	15
2.215	w	2.203	v w	2.21	30	2.22	10	2.21	10	2.204	10
2.125	w	2.127	m w	2.12	40	2.13	10	2.12	20	2.120	30
						2.11	10	2.11	5	2.099	10
				2.03	40	2.04	30	2.03	17	2.029	25
						2.02	10	2.01	10	2.006	15
1.970	w	1.969	m w	1.97	50	1.977	20	1.973	20	1.973	35
				1.94	30	1.943	20	1.939	15	1.938	20
		1.875	w			1.885	20	1.881	10	1.881	15
						1.865	10	1.859	10	1.859	10
1.832	w	1.833	w	1.83	40	1.843	10	1.833	15	1.833	20

+ 4 lines

+ 3 lines

+ 4 lines

1. Tenerite*, Pyörönmaa, Finland (this paper) (Debye-Scherrer method, camera diameter 57.3 mm, $\lambda = 1.5418 \text{ \AA}$)
2. Tenerite, Lövböle, Finland (this paper) (Debye-Scherrer method, camera diameter 57.3 mm, $\lambda = 1.5418 \text{ \AA}$)
3. Tenerite, Rosås, Norway (ASTM 16-698) ($\lambda = 1.93728$)
4. Tenerite, Iisaka, Japan (in Nagashima and Wakita, 1968) ($\lambda = 1.5405 \text{ \AA}$)
5. Synthetic yttrium carbonate (Nagashima and Wakita, 1968) ($\lambda = 1.5418 \text{ \AA}$)
6. Synthetic yttrium carbonate (this paper) (Philips wide-range X-ray diffractometer, $\lambda = 1.5418 \text{ \AA}$)

* Sample contaminated by lokkaite

All attempts to measure the density of lokkaite failed. The obtained results are too low due to adsorbed air.

Discussion

Tenerite from the type locality, Ytterby, Sweden, was poorly described (Svanberg and

Tenger, 1838) and later at least three different mineral species have been called tenerite. These »tengerites» resemble each other chemically, occur in the same way, and their indices of refraction are of the same order (Table 3), but they can be distinguished with certainty by X-ray methods (*cf.* Tables 2, 4 and 5).

The X-ray data of tenerite from Ytterby

are lacking but the X-ray powder pattern of tenerite from Rosås, Norway, checks with the material from Ytterby (Neumann and Bryn, 1958). The X-ray powder patterns of tenerites from Pyörönmaa and Lövböle*, Finland, Rosås, Norway, and Iisaka, Japan, are presented in Table 4. The comparison leaves no doubt that they represent one mineral species. It can be concluded that these data belong to tenerite.

The X-ray powder pattern of synthetic hydrous yttrium carbonate (Table 4) agrees with that of tenerite (Nagashima and Wakita, 1968). The idealized formula of the compound is $Y_2(CO_3)_3 \cdot 3H_2O$. The amount of water in the actual formula may be lower, as shown by the experiments of Nagashima and Wakita, in which case the average $Y_2O_3 : CO_2 : H_2O = 1.00 : 2.90 : 2.56$. The X-ray powder pattern of synthetic yttrium carbonate, supplied to the present author by K & K Laboratories, Inc., Plainview, N. Y. (Table 4), remains unchanged if run wet or dried at 110°C with the result that much of the contained water can be lost without any apparent change in the structure. According to Domingues *et al.* (1962) the weight loss at 110°C is about 7.5% and thus the actual formula is about $Y_2(CO_3)_3 \cdot 1.28 H_2O$. On the basis of the work done on the synthetic material it can be concluded, as stated by Nagashima and Wakita (1968), that the structure of tenerite is the same as that of hydrous yttrium carbonate. Though all published analyzed tenerites contain calcium, this element seems to be an unessential constituent in tenerite.

Stepanov (1961) has described a RE-carbonate from Kazakhstan, USSR, as tenerite. The X-ray powder pattern of this mineral is similar to that of the unidentified mineral of Verwoerd (1963) from Transvaal, South Africa, (Table 5) but quite different from that of tenerite (Table 4) and lokkaite (Table 2). According to Stepanov, the mineral is tetragonal with $a_0 = 8.375 \text{ \AA}$ and $c_0 = 8.72 \text{ \AA}$.

* Tenerite in Lövböle, Kemiö, SW-Finland, occurs as radial spheroids on gadolinite (Vorma *et al.*, 1966).

TABLE 5
X-ray powder patterns of two RE-carbonates

<i>hkl</i>	1.		2.	
	<i>d</i> (Å)	<i>I</i>	<i>d</i> (Å)	<i>I</i>
011	6.0	60	6.09	100
002	4.30	50	4.36	80
121	3.426	60	3.50	60
			3.31	30
			3.19	30
003	2.895	80	2.87	70
013	2.734	40	2.71	40
130	2.638	100	2.63	70
222	2.450	30	2.46	20
123	2.283	30	2.33	10
231	2.234	40	2.23	20
014	2.102	40	2.08	10
033	2.012	60	2.02	30
133	1.956	20		
240	1.871	100	1.88	90
340 } 050 }	1.672	40	1.65	20
	+ 5 lines		+ 2 lines	

1. »Tengerite», Kazakhstan, USSR. FeK, camera diameter 57.3 mm (Stepanov, 1961)
2. Unidentified RE-carbonate, Transvaal, South Africa. CoK, camera diameter 57.3 mm (Verwoerd, 1963)

Lokkaite was provisionally named tenerite (Vorma *et al.*, 1966) but later proved to be a new species. It mainly occurs intimately associated with tenerite. The mutual relationship of these two minerals is not known. Their X-ray powder patterns have much in common. All of the stronger reflections of tenerite, except in 7.6 Å, have one or two counterparts among the reflections of lokkaite, their *d*-values varying by a few hundredths of an Ångström unit (*cf.* Tables 2 and 4). It is improbable that the essential difference between lokkaite and tenerite is in the degree of hydration. The distinct superstructure in lokkaite suggests the presence of an order-disorder phenomenon, either substitutional (RE, Ca, vacancy) or rotational (CO_3^{2-}).

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