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FERROERICSSONITE, THE Fe²⁺ ANALOGUE OF ERICSSONITE, FROM EASTERN FRESNO COUNTY, CALIFORNIA, U.S.A.

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ABSTRACT

Ferroericssonite, ideally $\text{BaFe}^{2+}_2\text{Fe}^{3+}(\text{Si}_2\text{O}_7)\text{O(OH)}$, is a new mineral species found at both the Esquire #7 and #8 claims, situated along Big Creek in eastern Fresno County, and also at Trumbull Peak in Mariposa County, California, U.S.A. The mineral is the Fe²⁺ analogue of ericssonite and is named accordingly. Ferroericssonite crystallized very late in a sequence of minerals resulting from fluids interacting with a quartz–sanbornite vein along its margin with the country rock. It is closely associated with anandite, bazirite, celsian, devitoite, quartz and titanaramellite. The crystals occur in dark reddish brown foliated masses of irregular, undulating striated blades up to several mm in length, flattened on {100} and elongate and striated parallel to [001]. The mineral is transparent and has a brown streak, a vitreous luster, a Mohs hardness of approximately 4½, and two cleavages: {100} perfect and {011} good. It is brittle with an irregular fracture. The calculated densities are 4.445 and 4.413 g/cm³ on the basis of the empirical formulas for Esquire #7 and Esquire #8 material, respectively. It is optically biaxial (+), α 1.827(3), β 1.845(3), γ 1.920(6) (white light); $2V_{\text{meas}} = 63(2)^\circ$; $2V_{\text{cal}} = 63.0^\circ$; parallel dispersion, $r < v$; orientation: $X = \mathbf{b}$, $Y \approx \mathbf{c}$, $Z \approx \mathbf{a}$; pleochroic: brown, $Z > X > Y$. Electron-microprobe analyses of Esquire #7 and Esquire #8 material provided: BaO 30.11, 29.76, MgO 0.21, 0.10, MnO 1.19, 0.79, FeO 26.01, 26.24, Fe_2O_3 15.30, 15.35, Al_2O_3 0.02, 0.04, SiO_2 22.89, 23.34, F 0.09, 0.05, Cl 1.29, 0.88, H_2O 1.33, 1.42, F + Cl = O – 0.33, –0.22, total 98.11, 97.75 wt%, with FeO and Fe_2O_3 assignments and H_2O based on the structure. The empirical formulas for Esquire #7 and Esquire #8 material, based on Mg + Fe + Mn + Si = 5 apfu, are $\text{Ba}_{1.02}(\text{Fe}^{2+}_{1.89}\text{Mn}^{2+}_{0.09}\text{Mg}_{0.03})_{\Sigma 2.01}\text{Fe}^{3+}_{1.00}(\text{Si}_{1.99}\text{O}_7)\text{O}[(\text{OH})_{0.77}\text{O}_{0.02}\text{Cl}_{0.19}\text{F}_{0.02}]_{\Sigma 1}$ and $\text{Ba}_{1.01}(\text{Fe}^{2+}_{1.90}\text{Mn}^{2+}_{0.06}\text{Mg}_{0.01})_{\Sigma 1.97}\text{Fe}^{3+}_{1.00}(\text{Si}_{2.02}\text{O}_7)\text{O}[(\text{OH})_{0.82}\text{O}_{0.04}\text{Cl}_{0.13}\text{F}_{0.01}]_{\Sigma 1}$, respectively. Ferroericssonite is monoclinic, $C2/m$, a 20.3459(10), b 7.0119(3), c 5.3879(4) Å, β 94.874(7)°, V 765.89(7) Å³ and Z = 4. The strongest five lines in the X-ray powder-diffraction pattern [d_{obs} in Å(I)(hkl)] are: 3.708(42)(311), 3.506(81)(311, 510, 020), 2.880(42)(420), 2.788(100)(221) and 2.663(83)(202, 710). The crystal-structure determination ($R_1 = 3.56\%$ for 885 $F_o > 4\sigma F$) shows the mineral to be a heterophyllosilicate with a Fe²⁺ trioctahedral (O) sheet flanked on either side by heterophyllosilicate (H) layers, forming a HOH composite sheet. The heterophyllosilicate layers are composed of Si_2O_7 groups linked by Fe³⁺ square pyramids in a configuration referred to as a TS (Ti silicate) block, although five-coordinated Fe³⁺ takes the place of Ti⁴⁺. The region between the composite sheets is occupied by Ba²⁺. Ferroericssonite is a member of the lamprophyllite group.

Keywords: ferroericssonite, ericssonite, orthoericssonite, new mineral species, crystal structure, lamprophyllite group, heterophyllosilicate, TS block, Big Creek – Rush Creek sanbornite deposits, California.

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SOMMAIRE

La ferroericssonite, de composition idéale $\text{BaFe}^{2+}_2\text{Fe}^{3+}(\text{Si}_2\text{O}_7)\text{O(OH)}$, est une nouvelle espèce minérale découverte aux concessions minières Esquire #7 et #8, situées le long de Big Creek dans la partie orientale du comté de Fresno, et aussi au mont Trumbull, comté de Mariposa, en Californie, États-Unis. Le minéral est l'analogue Fe^{2+} de l'ericssonite, comme l'indique son nom. La ferroericssonite a cristallisé très tardivement dans une séquence de minéraux déposés à partir de fluides en interaction avec une veine de quartz + sanbornite et son encaissant. Elle est étroitement associée à anandite, bazirite, celsian, devitoïte, quartz et titanaramellite. On trouve les cristaux en amas feuilletés brun rougeâtre de lamelles irrégulières ondulantes atteignant une longueur de plusieurs mm, aplatis selon $\{100\}$ et allongés et striés parallèles à $[001]$. C'est un minéral transparent ayant une rayure brune, un éclat vitreux, une dureté de Mohs d'environ $4\frac{1}{2}$, et deux clivages, dont $\{100\}$ est parfait et $\{011\}$ est bon. Le minéral est cassant, avec une fracture irrégulière. Les densités calculées à partir des formules empiriques sont 4.445 et 4.413 g/cm^3 pour les échantillons provenant de Esquire #7 et Esquire #8, respectivement. La ferroericssonite est optiquement biaxe (+), $\alpha = 1.827(3)$, $\beta = 1.845(3)$, $\gamma = 1.920(6)$ (lumière blanche); $2V_{\text{mes}} = 63(2)^\circ$; $2V_{\text{calc}} = 63.0^\circ$; dispersion parallèle, $r < v$; orientation: $X = \mathbf{b}$, $Y \approx \mathbf{c}$, $Z \approx \mathbf{a}$; pleochroïque: brun, $Z > X > Y$. Les analyses effectuées avec une microsonde électronique ont donné, pour les échantillons Esquire #7 et Esquire #8: $\text{BaO } 30.11, 29.76$, $\text{MgO } 0.21, 0.10$, $\text{MnO } 1.19, 0.79$, $\text{FeO } 26.01, 26.24$, $\text{Fe}_2\text{O}_3 \ 15.30, 15.35$, $\text{Al}_2\text{O}_3 \ 0.02, 0.04$, $\text{SiO}_2 \ 22.89, 23.34$, $\text{F } 0.09, 0.05$, $\text{Cl } 1.29, 0.88$, $\text{H}_2\text{O } 1.33, 1.42$, $\text{F} + \text{Cl} \equiv \text{O } -0.33, -0.22$, pour un total de 98.11, 97.75% (poids), avec l'attribution de FeO et Fe_2O_3 et de H_2O conforme avec la structure. Les formules empiriques pour les échantillons Esquire #7 et Esquire #8, calculées sur une base de $\text{Mg} + \text{Fe} + \text{Mn} + \text{Si} = 5 \text{ apfu}$, sont $\text{Ba}_{1.02}(\text{Fe}^{2+}_{1.89}\text{Mn}^{2+}_{0.09}\text{Mg}_{0.03})\Sigma_{2.01}\text{Fe}^{3+}_{1.00}(\text{Si}_{1.99}\text{O}_7)\text{O}[(\text{OH})_{0.77}\text{O}_{0.02}\text{Cl}_{0.19}\text{F}_{0.02}]\Sigma_1$ et $\text{Ba}_{1.01}(\text{Fe}^{2+}_{1.90}\text{Mn}^{2+}_{0.06}\text{Mg}_{0.01})\Sigma_{1.97}\text{Fe}^{3+}_{1.00}(\text{Si}_{2.02}\text{O}_7)\text{O}[(\text{OH})_{0.82}\text{O}_{0.04}\text{Cl}_{0.13}\text{F}_{0.01}]\Sigma_1$, respectivement. La ferroericssonite est monoclinique, $C2/m$, $a = 20.3459(10)$, $b = 7.0119(3)$, $c = 5.3879(4) \text{ \AA}$, $\beta = 94.874(7)^\circ$, $V = 765.89(7) \text{ \AA}^3$ et $Z = 4$. Les cinq raies les plus intenses du spectre de diffraction X [d_{obs} en $\text{\AA}(I)(hkl)$] sont: 3.708(42)(311), 3.506(81)(311, 510, 020), 2.880(42)(420), 2.788(100)(221) et 2.663(83)(202, 710). Selon la détermination de la structure cristalline ($R_1 = 3.56\%$ pour 885 $F_o > 4\sigma F$), le minéral est un hétérophyllosilicate ayant un feuillet trioctaédrique (O) contenant Fe^{2+} , et sur chaque flanc, les couches hétérophyllosilicatées (H), le tout formant un feuillet composé HOH . Les couches hétérophyllosilicatées contiennent des groupes Si_2O_7 et des pyramides carrées renfermant le Fe^{3+} dans une configuration appelée bloc TS (silicate de Ti) dans lequel le Fe^{3+} joue le rôle de Ti^{4+} . Le Ba^{2+} occupe la région entre les feuillets composites. La ferroericssonite appartient au groupe de la lamprophyllite.

(Traduit par la Rédaction)

Mots-clés: ferroericssonite, ericssonite, orthoericssonite, nouvelle espèce minérale, structure cristalline, groupe de la lamprophyllite, hétérophyllosilicate, bloc TS, gisements de sanbornite de Big Creek – Rush Creek, Californie.

INTRODUCTION

The sanbornite deposits located along Big Creek and Rush Creek (Walstrom & Leising 2005) in Fresno County and at Trumbull Peak (Dunning & Cooper 1999) in Mariposa County, California, U.S.A. have now yielded 14 new mineral species, including ferroericssonite reported herein. This latest new species was discovered by one of the authors (GED) in 1998 at both the Esquire #7 and #8 claims on Big Creek and at Trumbull Peak. It was referred to in previous reports as mineral 39 and is closely associated with the recently described new mineral *devitoïte* (Kampf *et al.* 2010; IMA 2009–010).

The species is a member of the lamprophyllite group (Johnsen 1996) and is named as the Fe^{2+} analogue of ericssonite, $\text{BaMn}^{2+}_2\text{Fe}^{3+}(\text{Si}_2\text{O}_7)\text{O(OH)}$, (Moore 1971) in which Fe^{2+} takes the place of Mn^{2+} in the trioctahedral layer. The new mineral and name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2010–025). The two cotype specimens used in the description of the mineral are housed in the mineral collection of the Natural History Museum of Los Angeles County under catalogue numbers: 63206 (Esquire #7) and 63207 (Esquire #8).

OCCURRENCE

The mineral occurs at both the Esquire #7 and #8 claims along Big Creek, eastern Fresno County, California, U.S.A. The location of the Esquire #7 claim is SE $\frac{1}{4}$ SE $\frac{1}{4}$, Section 27, T11S, R25E, Mount Diablo Meridian; $36^{\circ}56'40''\text{N}$, $119^{\circ}14'28''\text{W}$, and that of the Esquire #8 claim is SE $\frac{1}{4}$ SW $\frac{1}{4}$, Section 22, T11S, R25E, Mount Diablo Meridian; $36^{\circ}56'42''\text{N}$, $119^{\circ}14'12''\text{W}$. The Esquire #7 and #8 claims were referred to by Walstrom & Leising (2005) as sites 6 and 5, respectively.

The mineral is found in a parallel-bedded quartz–sanbornite vein assemblage. It occurs along cleavage planes of altered gillespite and is closely associated with anandite, bazirite, celsian, devitoïte, quartz and titanaramellite. From textural relationships, ferroericssonite and devitoïte appear to be alteration products of gillespite. The parallel bedding also hosts the Fe^{3+} analogue of cerchiarite (currently under study), edingtonite, fresnoite, macdonaldite, pellyite, sanbornite, Ba-rich tobermorite, walstromite and witherite. The paragenetic position of the new mineral places it later than celsian, gillespite, sanbornite, titanaramellite and walstromite during a fluid interaction with the quartz–sanbornite vein along its margin with the country rock.

A description of the mineralogy of the sanbornite deposits along Big Creek and Rush Creek in eastern Fresno County, California, is provided by Walstrom & Leising (2005).

The mineral has also been found on a single sample of quartz–sanbornite rock from Trumbull Peak, Mariposa County, California (Dunning & Cooper 1999).

PHYSICAL AND OPTICAL PROPERTIES

Ferroericssonite crystals (Fig. 1) occur in dark reddish brown foliated masses of irregular, undulating striated blades to several mm in length, flattened on {100} and elongate and striated parallel to [001]. No twinning was observed. The streak is brown. Crystals

are transparent with a vitreous luster. The mineral is brittle with an irregular fracture and a Mohs hardness of approximately 4½. It has two cleavages: {100} perfect and {011} good. The density exceeds those of available liquids, and there is insufficient material for direct measurement. The calculated densities are 4.425 g/cm³ based on the structural formula, 4.445 g/cm³ based on the empirical formula for Esquire #7 material, and 4.413 g/cm³ based on the empirical formula for Esquire #8 material. Crystals react very slowly in dilute or concentrated HCl, forming a colorless residue.

The mineral is optically biaxial (+), with the following optical constants measured in white light: α 1.827(3), β 1.845(3), γ 1.920(6). The measured $2V$ is 63(2)°, and the calculated $2V$ is 63.0°. The dispersion is parallel, $r < v$; The optical orientation is $X = \mathbf{b}$; $Y \approx \mathbf{c}$; $Z \approx \mathbf{a}$, and the pleochroism is brown, $Z > X > Y$.

CHEMICAL COMPOSITION

Chemical analyses (18 for Esquire #7 and 11 for Esquire #8) were carried out by means of a Cameca SX-50 electron microprobe outfitted with four wavelength-dispersion spectrometers (WDS mode, 15 kV, 10 nA, 5 µm beam diameter). Acquisition time was 10 s on peak and 5 s on low and high background positions. Data reduction was accomplished with a ZAF matrix correction (Armstrong 1988) using Probe for Windows software. The small amount of material available did not allow for the direct determination of H₂O, so it was calculated from the structure. The FeO and Fe₂O₃ are also allocated in accord with the structure. Analytical data are given in Table 1.

The empirical formulas for Esquire #7 and Esquire #8 material, based on five cations in the layer portion of the structure (Mg + Fe + Mn + Si =

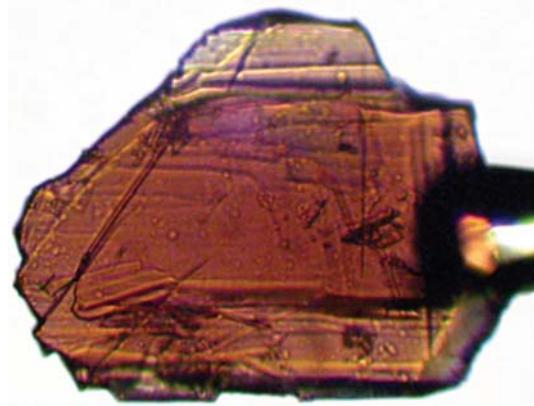


FIG. 1. Dark reddish brown fragment of a ferroericssonite crystal (0.21 × 0.14 × 0.01 mm) used in the optical study.

TABLE 1. ANALYTICAL MICROPROBE RESULTS FOR FERROERICSSONITE

Const.	Esquire #7			Esquire #8			
	wt%	Range	SD	wt%	Range	SD	Probe standard
BaO	30.11	28.44–31.62	0.99	29.76	28.89–30.73	0.61	sanbornite
MgO	0.21	0.14–0.23	0.02	0.10	0.05–0.13	0.02	enstatite
FeO	39.85	38.67–40.65	0.54	40.02	39.25–40.95	0.64	forsterite-80
MnO	1.19	1.02–1.32	0.08	0.79	0.65–0.88	0.08	rhodonite
Al ₂ O ₃	0.02	0.00–0.09	0.03	0.04	0.00–0.12	0.05	kyanite
SiO ₂	22.89	22.00–23.95	0.59	23.34	23.03–23.70	0.22	kyanite
F	0.09	0.00–0.38	0.15	0.05	0.00–0.28	0.11	fluorite
Cl	1.29	1.12–1.54	0.12	0.88	0.63–1.04	0.12	KCl
H ₂ O*	1.33		1.42				
F+Cl=O	-0.33		-0.22				
FeO*	26.01		26.24				
Fe ₂ O ₃ *	15.30		15.35				
Total	98.11		97.75				

* H₂O, FeO and Fe₂O₃ assignments are based on the structure.

5 *apfu*), are $\text{Ba}_{1.02}(\text{Fe}^{2+})_{1.89}\text{Mn}^{2+}_{0.09}\text{Mg}_{0.03})\Sigma_{2.01}\text{Fe}^{3+}_{1.00}(\text{Si}_{1.99}\text{O}_7)\text{O}[(\text{OH})_{0.77}\text{O}_{0.02}\text{Cl}_{0.19}\text{F}_{0.02}]\Sigma_1$ and $\text{Ba}_{1.01}(\text{Fe}^{2+})_{1.90}\text{Mn}^{2+}_{0.06}\text{Mg}_{0.01})\Sigma_{1.97}\text{Fe}^{3+}_{1.00}(\text{Si}_{2.02}\text{O}_7)\text{O}[(\text{OH})_{0.82}\text{O}_{0.04}\text{Cl}_{0.13}\text{F}_{0.01}]\Sigma_1$, respectively. The simplified formula is $\text{BaFe}^{2+}_2\text{Fe}^{3+}(\text{Si}_2\text{O}_7)\text{O}(\text{OH})$, which requires 30.30 BaO, 28.40 FeO, 15.78 Fe₂O₃, 23.75 SiO₂, 1.78 H₂O, for a total of 100.00 wt%.

The Gladstone–Dale compatibility index 1 – (K_p/K_C), as defined by Mandarino (1981), provides a measure of the consistency among the average index of refraction, calculated density and chemical composition. For ferroericssonite, the compatibility index is –0.0126 (superior) based on the structural formula, –0.0131 (superior) based on the Esquire #7 empirical

formula and –0.0214 (excellent) based on the Esquire #8 empirical formula.

X-RAY CRYSTALLOGRAPHY AND STRUCTURE DETERMINATION

Both powder and single-crystal X-ray studies were carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with monochromatized MoK α radiation. For the powder-diffraction study, observed values of d and intensities were derived by profile fitting using JADE 9.1 software. The powder data presented in Table 2 show good agreement with the pattern calculated from the structure determination. Unit-cell parameters refined from the powder data using JADE 9.1 with whole pattern fitting are: a 20.395(13), b 7.025(13), c 5.389(13) Å, β 94.872(17) $^\circ$ and V 769(2) Å³.

The Rigaku CRYSTALCLEAR software package was used for processing the structure data, including the application of a numerical (shape-based) absorption correction. The structure was solved by direct methods using SIR92 (Altomare *et al.* 1994), and the location of all non-hydrogen atoms was straightforward. SHELXL-97 (Sheldrick 2008) was used for the refinement of the structure. For a crystal from the Esquire #8 claim, with all atoms refined anisotropically, the refinement converged to $R_1 = 3.56\%$ and $wR_2 = 8.58\%$ for 885 reflections with $F_o > 4\sigma F$. Similar results ($R_1 = 3.93\%$ for 835 $F_o > 4\sigma F$ reflections) were obtained for a crystal from the Esquire #7 claim. The details of the data collection and the final refinement of the structure for the Esquire #8 crystal are provided in Table 3. Note that relatively high electron-density residuals are probably best interpreted as due to some order-disorder, perhaps related to the presence of a small amount of the orthorhombic polytype (as was noted for ericssonite–orthoericssonite; Moore 1971). There is some streaking evident in the single-crystal frames that supports this interpretation. The Cl indicated in the electron-microprobe analyses is apparently accommodated at the O1 site, as indicated by the refined site-occupancy and the relatively high displacement-parameters for the site. The final coordinates and displacement parameters of atoms are provided in Table 4. Selected interatomic distances are listed in Table 5, and bond valences, in Table 6. Tables of observed and calculated structure-factors are available from the Depository of Unpublished data on the Mineralogical Association of Canada website [document Ferroericssonite CM49_587].

ATOMIC ARRANGEMENT

Ferroericssonite has a heterophyllosilicate structure (Fig. 2) with a Fe^{2+} trioctahedral (O) sheet flanked on either side by heterophyllosilicate (H) layers, forming a HOH composite sheet (Ferraris *et al.* 1996, 2008, Ferraris 2008). The heterophyllosilicate layers are

TABLE 2. X-RAY POWDER-DIFFRACTION DATA FOR FERROERICSSONITE

	I_{obs}	d_{obs}	d_{calc}	I_{calc}	h	k	l	I_{obs}	d_{obs}	d_{calc}	I_{calc}	h	k	l
18	5.0977	5.0681	10	4	0	0	3	1.8688	1.8686	10	5	3	1	
26	4.1477	4.2292	7	7	1	1		1.8454	5	10	0	1		
	4.1158	14	1	1	1		7	1.8205	1.8251	11	7	1	3	
42	3.7079	3.7203	40	3	1	1		1.8188	14	7	3	0		
	3.5383	6	4	0	1			1.7824	5	11	1	0		
	3.5099	14	5	1	0		29	1.7534	1.7530	47	0	4	1	
81	3.5058	3.5060	10	0	2	0		1.7457	9	9	1	2		
	3.5003	47	3	1	1		5	1.7132	1.7156	5	1	1	3	
18	3.3880	3.3787	19	6	0	0		1.7138	6	3	1	3		
23	3.3202	3.3134	19	2	2	0		1.6907	1.6882	17	10	0	2	
38	3.0269	3.0420	46	5	1	1		1.6567	6	4	4	0		
	2.9758	9	6	0	1			1.6472	15	3	1	3		
	2.9354	5	0	2	1		43	1.6412	1.6439	14	5	1	3	
42	2.8797	2.8833	19	4	2	0		1.6330	53	10	2	1		
	2.8552	7	2	2	1			1.5939	26	0	2	3		
	2.8435	38	5	1	1		36	1.5919	1.5931	27	2	2	3	
100	2.7884	2.7852	100	2	2	1		1.5845	8	5	3	2		
	2.7559	9	6	0	1			1.5554	5	10	0	2		
	2.6842	9	0	0	2			1.5488	6	5	1	3		
83	2.6626	2.6767	36	7	1	0		1.5461	1.5448	6	7	1	3	
	2.6511	42	2	0	2		15	1.5445	16	7	3	2		
23	2.5996	2.5929	30	4	2	1		1.4927	1.4945	50	12	2	1	
	2.5419	8	2	0	2			1.4885	8	4	2	3		
15	2.5344	2.5340	12	8	0	0		1.4879	6	12	0	2		
	2.4904	8	4	2	1			1.4856	8	6	2	3		
	2.4743	9	7	1	1			1.4791	5	6	4	1		
18	2.4521	2.4601	7	4	0	2		1.4697	17	7	3	2		
	2.4329	9	6	2	0		29	1.4638	1.4677	9	0	4	2	
2	2.3762	2.3706	7	8	0	1		1.4622	30	2	4	2		
2	2.2908	2.2917	4	3	1	2		1.4480	10	14	0	0		
	2.2199	7	8	0	1		12	1.4419	1.4431	7	2	4	2	
18	2.2035	2.2121	9	5	1	2		1.4416	11	8	4	0		
	2.1945	20	6	0	2			1.4274	11	-9	3	2		
22	2.1609	2.1667	28	6	2	1		1.4108	5	1	3	3		
	2.1445	16	9	1	0		5	1.4108	1.4097	5	3	3		
	2.1387	9	7	3	1			1.4095	5	8	4	1		
	2.1313	30	0	2	2			1.3708	17	12	0	2		
55	2.1263	2.1236	5	1	3	1		1.3747	1.3719	5	3	3		
	2.1146	25	2	2	2		11	1.3701	5	5	3	3		
	2.0630	9	3	3	1			1.3696	7	6	4	2		
25	2.0575	2.0603	15	5	1	2		1.3455	6	2	0	4		
	2.0579	13	2	2	2		17	1.3409	1.3421	17	0	0	4	
	2.0249	20	5	3	0			1.3358	8	3	5	1		
37	2.0229	2.0231	16	3	3	1		9	1.3234	1.3248	8	3	5	1
	2.0198	15	6	0	2			1.3239	6	6	4	2		
	2.0138	8	4	2	2		14	1.3038	1.3054	11	8	2	3	
15	1.9683	1.9745	14	7	1	2		1.3017	12	10	2	3		
	1.9638	18	8	2	1			1.2972	5	13	3	0		
	1.9521	6	10	0	1			1.2951	8	5	5	1		
6	1.9237	1.9217	17	5	3	1		4	1.2809	1.2785	9	5	5	1

TABLE 3. FERROERICSSONITE: DETAILS ON DATA COLLECTION AND THE STRUCTURE REFINEMENT

Locality	Esquire #8 claim, Big Creek, Fresno County, California
Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation / power	MöKa ($\lambda = 0.71075 \text{ \AA}$) / 50 kV, 40 mA
Temperature	298(2) K
Structural formula	$\text{BaFe}^{3+}_2\text{Fe}^{3+}(\text{Si}_2\text{O}_7)\text{O(OH)}_{0.77}\text{Cl}_{0.23}$
Space group	$C2/m$
Unit-cell parameters	
a, b	20.3459(10), 7.0119(3) Å
c, β	5.3879(4) Å, 94.874(7) $^\circ$
Z	4
Volume	765.89(7) Å ³
Density (for structural formula)	4.419 g/cm ³
Absorption coefficient	11.062 mm ⁻¹
$F(000)$	944
Crystal size	80 × 70 × 15 μm
θ range	3.07 to 27.48 $^\circ$
Index ranges	-26 ≤ h ≤ 26, -9 ≤ k ≤ 9, -6 ≤ l ≤ 6
Reflections collected / unique	5834 / 937 [$R_{\text{int}} = 0.0364$]
Reflections with $F_o > 4\sigma F$	885
Completeness to $\theta = 27.48^\circ$	99.2%
Max. and min. transmission	0.8516 and 0.4715
Refinement method	Full-matrix least-squares on F^2
Parameters refined	81
GoF	1.083
Final R indices [$F_o > 4\sigma F$]	$R_1 = 0.0356$, $wR_2 = 0.0858$
R indices (all data)	$R_1 = 0.0371$, $wR_2 = 0.0871$
Extinction coefficient	0.00036(11)
Largest diff. peak / hole	+4.509 / -0.887 e/Å ³

Notes: $R_{\text{int}} = \sum |F_o|^2 - |F_c|^2 (\text{mean})| / \sum |F_c|^2$. GoF = $S = \{\sum [w(F_o^2 - F_c^2)^2] / (n-p)\}^{1/2}$. $R_1 = \sum |F_o| - |F_c| / \sum |F_c|$. $wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_c^2)]\}^{1/2}$, $w = 1/[a^2(F_o^2) + (aP)^2 + bP]$, where a is 0.0667, b is 2.2304, and P is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$.

composed of Si_2O_7 groups linked by Fe^{3+} square pyramids (Fig. 3) in a configuration referred to by Sokolova (2006) as a TS (Ti silicate) block, although in ferroericssonite (as in orthoericssonite, Fig. 2; Matsubara 1980), five-coordinated Fe^{3+} takes the place of Ti^{4+} . The region between the composite sheets is occupied by Ba^{2+} .

POLYTYPE NOMENCLATURE FOR ERICSSONITE AND ORTHOERICSSONITE

The structure of ericssonite has not been determined, but ericssonite can be assumed to be isostructural with ferroericssonite. The structures of ferroericssonite (monoclinic, $C2/m$) and orthoericssonite (orthorhombic, $Pnnm$) are compared in Figure 2. The difference between the structures involves different orientations of successive HOH layers. In the monoclinic structure, all HOH layers are in the same orientation, whereas in the orthorhombic structure, alternate layers are flipped relative to one another. Therefore, ericssonite and orthoericssonite are polytypes and should be properly named ericssonite- $2M$ and ericssonite- $2O$, respectively, in accord with the polytype nomenclature introduced by Johnsen (1996) for the lamprophyllite group. This is analogous to the polytypes lamprophyllite- $2M$ and lamprophyllite- $2O$ (Krivovichev *et al.* 2003) and the

TABLE 4. COORDINATES AND DISPLACEMENT PARAMETERS (Å²) OF ATOMS IN FERROERICSSONITE

	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba	0.225048(16)	0.0000	0.24144(6)	0.00956(18)	0.0113(2)	0.0081(3)	0.0093(3)	0.000	0.00105(15)	0.000
Fe1	0.0000	0.26153(13)	0.0000	0.0121(2)	0.0150(5)	0.0126(5)	0.0091(5)	0.000	0.0033(4)	0.000
Fe2	0.0000	0.0000	0.5000	0.0124(3)	0.0147(6)	0.0118(6)	0.0106(6)	0.000	0.0004(5)	0.000
Fe3	0.0000	0.5000	0.5000	0.0107(3)	0.0139(6)	0.0106(6)	0.0082(6)	0.000	0.0038(5)	0.000
Fe4	0.14026(4)	0.5000	0.21580(16)	0.0068(2)	0.0088(4)	0.0060(4)	0.0057(4)	0.000	0.0007(3)	0.000
Si	0.13431(6)	0.22566(16)	0.7125(2)	0.0062(3)	0.0086(6)	0.0052(5)	0.0047(5)	0.0002(4)	0.0002(4)	0.0005(4)
O1*	0.0555(3)	0.0000	0.1802(8)	0.038(2)	0.073(4)	0.025(3)	0.017(3)	0.000	0.006(2)	0.000
O2	0.1574(2)	0.0000	0.7195(9)	0.0126(9)	0.012(2)	0.006(2)	0.019(2)	0.000	0.0021(17)	0.000
O3	0.05466(16)	0.2455(4)	0.6846(6)	0.0099(6)	0.0085(14)	0.0111(15)	0.0101(15)	-0.0008(11)	0.0015(12)	0.0015(11)
O4	0.16858(15)	0.3090(5)	0.9732(6)	0.0105(6)	0.0135(15)	0.0103(14)	0.0076(13)	-0.0007(11)	0.0008(11)	-0.0005(11)
O5	0.16897(15)	0.3092(4)	0.4761(6)	0.0105(6)	0.0125(14)	0.0105(14)	0.0086(14)	0.0028(11)	0.0013(11)	0.0007(11)
O6	0.0497(2)	0.5000	0.1922(8)	0.0101(8)	0.009(2)	0.011(2)	0.010(2)	0.000	0.0030(16)	0.000

* The refined occupancy of the O1 site is (OH): 0.77(2) and Cl: 0.23(2).

TABLE 5. SELECTED BOND-DISTANCES (Å) IN FERROERICSSONITE

Ba–O4 (x2)	2.796(3)	Fe1–O3 (x2)	2.111(3)	Fe3–O6 (x2)	2.015(4)	Si–O5	1.618(3)
Ba–O5 (x2)	2.801(3)	Fe1–O6 (x2)	2.171(3)	Fe3–O3 (x4)	2.286(3)	Si–O3	1.621(3)
Ba–O5 (x2)	2.863(3)	Fe1–O1 (x2)	2.323(3)	<Fe3–O>	2.196	Si–O4	1.623(3)
Ba–O4 (x2)	2.871(3)	<Fe1–O>	2.202			Si–O2	1.650(2)
Ba–O2	3.022(5)			Fe4–O6	1.836(5)	<Si–O>	1.628
Ba–O2	3.024(5)	Fe2–O1 (x2)	2.139(5)	Fe4–O5 (x2)	1.989(3)		
<Ba–O>	2.871	Fe2–O3 (x4)	2.236(3)	Fe4–O4 (x2)	1.991(3)		
		<Fe2–O>	2.204	<Fe4–O>	1.959		

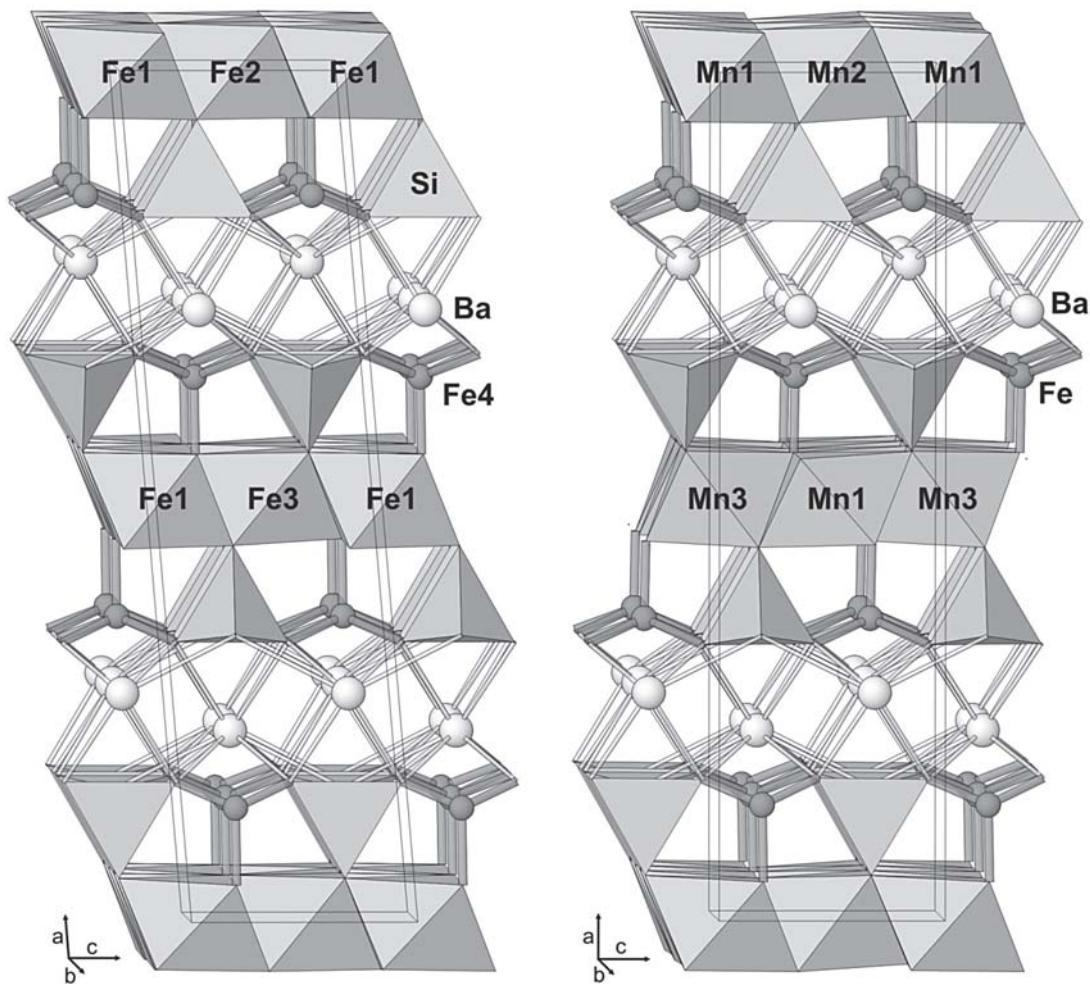


FIG. 2. Structures of ferroericssonite (left) and orthoericssonite (right). Square pyramidal Fe^{3+}O_5 coordination is shown in "ball-and-stick" form to distinguish it from the SiO_4 tetrahedra. Note the different orientations of the Fe^{2+}O_6 and Mn^{2+}O_6 octahedra in the trioctahedral sheets at $x = \frac{1}{2}$.

polytypes nabalamprophyllite- $2M$ (Rastsvetaeva & Chukanov 1999) and nabalamprophyllite- $2O$ (Sokolova & Hawthorne 2008), which in each case are isotopic with ericssonite and orthoericssonite, respectively. If the orthorhombic polytype of ferroericssonite is found, the monoclinic and orthorhombic polytypes should be named using the same polytype suffix approach, *i.e.*, ferroericssonite- $2M$ and ferroericssonite- $2O$. Finally, if the orthorhombic polytype of barytolamprophyllite is found, the monoclinic and orthorhombic polytypes should be named using the same polytype suffix approach, *i.e.*, barytolamprophyllite- $2M$ and barytolamprophyllite- $2O$.

Note that because polytypes are not considered as distinct mineral species, the renaming of orthoericssonite to ericssonite- $2O$ implies a discredititation of orthoericssonite. The renaming of ericssonite and orthoericssonite to ericssonite- $2M$ and ericssonite- $2O$, respectively, and the discredititation of orthoericssonite as a distinct species, have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (Nomenclature Voting Proposal 10-F). Table 7 lists all of the currently accepted minerals (and polytypes) in the lamprophyllite group.

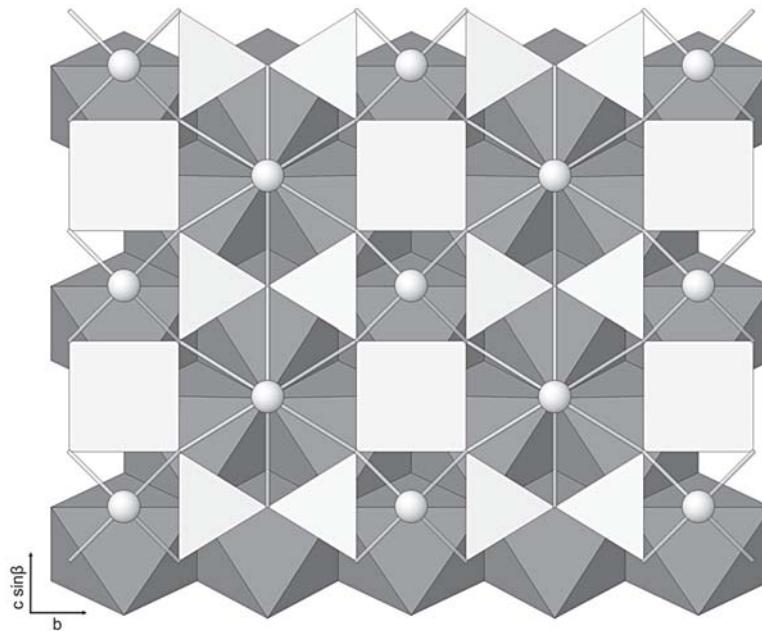


FIG. 3. Ferroericssonite structure viewed parallel to {100} showing linkage of Si_2O_7 groups (white triangles) and Fe^{3+}O_5 square pyramids (white squares) in the heterophyllosilicate layers. The Ba atoms are shown as white spheres. The Fe^{2+}O_6 octahedra in the trioctahedral layer are shown in gray.

TABLE 6. BOND-VALENCE ANALYSIS FOR FERROERICSSONITE

	Ba	Fe1	Fe2	Fe3	Fe4	Si	Sum
O1*		0.249 ^{*21}	0.410 ^{*21}				0.908
O2	0.136 ^{*21}					0.932 ^{*2-}	2.136
O3		0.361 ^{*21}	0.257 ^{*41}	0.225 ^{*41}		1.008	1.852
O4	0.251 ^{*21}				0.534 ^{*21}	1.003	1.993
O5	0.205 ^{*21}				0.537 ^{*21}	1.016	2.011
O6	0.248 ^{*21}				0.210 ^{*21}		
		0.307 ^{*21}		0.468 ^{*21}	0.812		1.894
Sum	2.100	1.834	1.850	1.836	2.955	3.959	

Notes: Multiplicity is indicated by $\times -1$; $\text{Ba}^{2+}-\text{O}$, $\text{Fe}^{2+}-\text{O}$ and $\text{Fe}^{3+}-\text{O}$ bond strengths from Brown & Altermatt (1985); $\text{Fe}^{2+}-\text{Cl}$ bond strength from Brese & O'Keeffe (1991); bond strength for the O1 site is assigned in accord with refined site-occupancy $[(\text{OH})_{0.77}\text{Cl}_{0.23}]$. Values are expressed in valence units.

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TABLE 7. MEMBERS OF THE LAMPROPHYLLITE GROUP

Mineral species	Ideal formula	Space group
lamprophyllite-2M	(SrNa)(Na ₃ Ti ⁴⁺)Ti ⁴⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	C2/m
lamprophyllite-2O	(SrNa)(Na ₃ Ti ⁴⁺)Ti ⁴⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	Pnmm
nabalampophyllite-2M	(BaNa)(Na ₃ Ti ⁴⁺)Ti ⁴⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	P2/m
nabalampophyllite-2O	(BaNa)(Na ₃ Ti ⁴⁺)Ti ⁴⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	Pnmm
barytolamprophyllite	(BaK)(Na ₃ Ti ⁴⁺)Ti ⁴⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	C2/m
ericssonite-2M *	Ba ₂ Mn ²⁺ Fe ³⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	C2/m
ericssonite-2O **	Ba ₂ Mn ²⁺ ₄ Fe ³⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	Pnmm
ferroericssonite	Ba ₂ Fe ²⁺ ₄ Fe ³⁺ ₂ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	C2/m

* formerly ericssonite; ** formerly orthoericssonite. Note that the formulas provided for ericssonite-2M and ericssonite-2O are for Z = 2, rather than Z = 4, in order to conform with the formulas for the other members.

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