FERROKENTBROOKSITE, A NEW MEMBER OF THE EUDIALYTE GROUP FROM MONT SAINT-HILAIRE, QUEBEC, CANADA

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Abstract

Ferrokentbrooksite, ideally $Na_{15}Ca_6(Fe,Mn)_3Zr_3NbSi_{25}O_{73}(O,OH,H_2O)_3(Cl,F,OH)_2$, is a new member of the eudialyte group from Mont Saint-Hilaire, Quebec; it is the ferrous-iron-dominant analogue of kentbrooksite. It occurs as reddish brown to red, pseudo-octahedral crystals to 1 cm in diameter. Associated minerals include microcline, nepheline (partially altered to natrolite), fluorite, fluorapatite, natrolite, gonnardite, rhodochrosite, aegirine, albite, calcite, sérandite, ancylite-(Ce), and catapleiite. It is transparent with a vitreous luster and a white streak. It is brittle, with a hardness of 5–6 (Mohs scale). It has no cleavage, no parting, and an uneven to conchoidal fracture. It is uniaxial negative with ω 1.6221(3) and ε 1.6186(3). It is trigonal, space group $R3m$, a 14.2099(7) and c 30.067(2) Å, V 5257.7(3) Å^3, $Z = 3$. The strongest nine X-ray powder-diffraction lines [d in Å(I)(hkl)] are: 7.104(38)(110), 5.694(50)(202), 4.300(43)(205), 3.955(31)(214), 3.391(51)(131), 3.207(31)(208), 3.155(31)(217), 2.968(100)(315) and 2.847(98)(404). The infrared spectrum of ferrokentbrooksite is given. An average result of two electron-microprobe analyses of the grain on which the structure was refined gave Na_2O 11.96, K_2O 0.44, CaO 7.99, MnO 3.88, FeO 5.08, SrO 0.45, Al_2O_3 0.11, Y_2O_3 0.58, La_2O_3 1.51, Ce_2O_3 2.51, Nd_2O_3 0.53, Sm_2O_3 0.11, Gd_2O_3 0.17, SiO_2 44.70, TiO_2 0.09, ZrO_2 11.20, HfO_2 0.17, Nb_2O_5 2.51, Ta_2O_5 0.16, F 0.40, Cl 0.93, H_2O 0.35, O ≡ F, Cl –0.38, for a total of 95.45 wt.%. The amount of H_2O was calculated by stoichiometry from the crystal-structure analysis. The empirical formula of ferrokentbrooksite, based on 77.47 anions as determined in the crystal-structure analysis, is: $(Na_{13.05}REE_{0.99}K_{0.32}Ca_{0.23}Sr_{0.15})_{\Sigma14.74}(Ca_{4.59}Mn_{1.24}Y_{0.17})_{\Sigma6}$ $(Fe_{2.39}Mn_{0.61})_{\Sigma3}(Zr_{3.00}Ti_{0.04}Hf_{0.03})_{\Sigma3.07}(Nb_{0.64}Si_{0.23}Zr_{0.07}Ta_{0.02})_{\Sigma0.96}(Si_{24.93}Al_{0.07})_{\Sigma25}O_{73}(O,OH,H_2O)_{\Sigma2.47}(Cl_{0.89}F_{0.71}OH_{0.40})_{\Sigma2}$; $D_{meas} = 3.06(3)$ g/cm^3, $D_{calc} = 3.06$ g/cm^3. Ferrokentbrooksite possesses the eudialyte structure, and has Fe as the predominant element at $M(2)$ replacing Mn. Fe is predominantly five-fold coordinated, and bond-valence calculations indicate it to be divalent.

Keywords: ferrokentbrooksite, eudialyte, new mineral species, crystal structure, Mont Saint-Hilaire, Quebec.

Sommaire

La ferrokentbrooksite, dont la formule idéale est $Na_{15}Ca_6(Fe,Mn)_3Zr_3Nb\,Si_{25}O_{73}(O,OH,H_2O)_3(Cl,F,OH)_2$, est un nouveau membre du groupe de l'eudialyte découvert au mont Saint-Hilaire, Québec; il s'agit de l'analogue de la kentbrooksite à dominance de Fe^{2+}. Elle se présente en cristaux pseudo-octaédriques brun-rouge à rouge, atteignant 1 cm de taille. Lui sont associés microcline, néphéline (partiellement transformée en natrolite), fluorite, fluorapatite, natrolite, gonnardite, rhodochrosite, aegyrine, albite, calcite, sérandite, ancylite-(Ce), et catapléiite. Le minéral est transparent, avec un éclat vitreux et une rayure blanche; il est cassant, avec une dureté de Mohs de 5 à 6. Il n'y a aucun clivage ou plan de séparation, et la fracture est inégale à conchoïdale. La ferrokentbrooksite est uniaxe négative, avec ω 1.6221(3) et ε 1.6186(3). Elle est trigonale, groupe spatial $R3m$, a 14.2099(7) et c 30.067(2) Å, V 5257.7(3) Å^3, $Z = 3$. Les neuf raies les plus intenses du spectre de diffraction X (méthode des poudres) [d en Å(I)(hkl)] sont: 7.104(38)(110), 5.694(50)(202), 4.300(43)(205), 3.955(31)(214), 3.391(51)(131), 3.207(31)(208), 3.155(31)(217), 2.968(100)(315) et 2.847(98)(404). Nous présentons le spectre infrarouge de la ferrokentbrooksite. Les analyses à la microsonde électronique du cristal ayant servi pour l'ébauche de la structure ont donné, en moyenne, Na_2O 11.96, K_2O 0.44, CaO 7.99, MnO 3.88, FeO 5.08, SrO 0.45, Al_2O_3 0.11, Y_2O_3 0.58, La_2O_3 1.51, Ce_2O_3 2.51, Nd_2O_3 0.53, Sm_2O_3 0.11, Gd_2O_3 0.17, SiO_2 44.70, TiO_2 0.09, ZrO_2 11.20, HfO_2 0.17, Nb_2O_5 2.51, Ta_2O_5 0.16, F 0.40, Cl 0.93, H_2O 0.35, O ≡ F, Cl –0.38, pour un total de 95.45% (poids). La quantité de H_2O a été calculée par stoichiométrie selon les résultats de l'étude structurale. La formule empirique de la ferrokentbrooksite, fondée sur 77.47 anions, tel qu'indiqué par les résultats structuraux, est: $(Na_{13.05}TR_{0.99}K_{0.32}Ca_{0.23}Sr_{0.15})_{\Sigma14.74}(Ca_{4.59}Mn_{1.24}Y_{0.17})_{\Sigma6}(Fe_{2.39}Mn_{0.61})_{\Sigma3}(Zr_{3.00}Ti_{0.04}Hf_{0.03})_{\Sigma3.07}(Nb_{0.64}Si_{0.23}Zr_{0.07}Ta_{0.02})_{\Sigma0.96}(Si_{24.93}Al_{0.07})_{\Sigma25}O_{73}(O,OH,H_2O)_{\Sigma2.47}(Cl_{0.89}F_{0.71}OH_{0.40})_{\Sigma2}$; $D_{mes} = 3.06(3)$, $D_{calc} = 3.06$ g/cm^3. La ferrokentbrooksite possède la structure de l'eudialyte,

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avec Fe comme occupant principal du site *M*(2) en remplacement de Mn. Le Fe est surtout en coordinence cinq, et d'après un calcul des valences de liaisons, serait bivalent.

(Traduit par la Rédaction)

Mots-clés: ferrokentbrooksite, eudialyte, nouvelle espèce minérale, structure cristalline, mont Saint-Hilaire, Québec.

INTRODUCTION

During a systematic study of the chemical composition of the Na-rich zirconosilicate eudialyte (Johnsen & Gault 1997), several private collectors contributed numerous specimens, which enabled us to sample a broad spectrum of eudialyte-group minerals from various occurrences. One of these specimens, sent to us by László and Elsa Horváth of Hudson, Quebec, proved to be the ferrus-iron-dominant analogue of kentbrooksite and a new member of the eudialyte group. This sample, which has become the holotype specimen of the new species ferrokentbrooksite, was collected from the Poudrette Quarry, Mont Saint-Hilaire, Rouville County, Quebec in 1992. The purpose of this paper is to describe this new member of the eudialyte group, its structure and occurrence.

The new mineral and its name have been approved by the Commission on New Minerals and Mineral Names (CNMMN), IMA (IMA# 99–046). The name is in keeping with the recommendations of the Subcommittee on Eudialyte Nomenclature of the CNMMN (Johnsen *et al.*, in prep.). One of the recommendations of the Subcommittee is that the anion site be ignored in general, in terms of the nomenclature of this group; this recommendation has been followed in this case. The holotype specimen (catalogue no. CMNMC 81563) is housed in the collection of the Canadian Museum of Nature, Ottawa.

OCCURRENCE

Mont Saint-Hilaire is an alkaline intrusive complex and one of the ten Monteregian Hills, a series of genetically related plutons that are aligned along the St. Lawrence Valley for almost 250 km eastward from Oka to Megantic in the province of Quebec. The complexity of the Mont Saint-Hilaire pluton is reflected in the wide variation in chemical composition of the eudialyte-group minerals from this locality (Johnsen & Gault 1997). In addition to ferrokentbrooksite, five other members of the eudialyte group, namely eudialyte *sensu stricto* (*s.s.*), kentbrooksite (Johnsen *et al.* 1998), khomyakovite and manganokhomyakovite (Johnsen *et al.* 1999a) and oneillite (Johnsen *et al.* 1999b) have been identified from the numerous geological mini-environments at Mont Saint-Hilaire (Horváth & Gault 1990).

The mineral formed as a primary but late-stage phase in a small pegmatite dyke in nepheline syenite, exposed during quarrying operations. Some hydrothermal alteration of the dyke rocks has occurred, as indicated in back-scattered electron imaging. The ferrokentbrooksite has remained quite fresh except for a thin, glaze-like alteration to catapleiite along the surface. Mineral species associated with ferrokentbrooksite in the pegmatite are microcline, nepheline (partially altered to natrolite), fluorite, fluorapatite, natrolite, gonnardite, rhodochrosite, aegirine, albite, calcite, sérandite, ancylite-(Ce), and catapleiite.

In addition to the holotype specimen, a number of other analyzed specimens from Mont Saint-Hilaire have proven to be ferrokentbrooksite, making this species at least as common as eudialyte *s.s.* at this locality. In addition to being found in several other agpaitic pegmatite dykes, including the informally designated Poudrette pegmatite, a relatively large (2 to 4 m across) dyke which has been exposed on four levels of the quarry, it has also been found as a late-stage magmatic mineral in miarolitic cavities in the nepheline syenite, as a rock-forming mineral in the nepheline syenite itself, and in igneous breccia. Ferrokentbrooksite has also been identified from the Narssârssuk Pegmatite, Igaliko alkaline complex in southwestern Greenland, in the Langesundfjord area, Norway (at Brønnebukta, Siktesøya; Barkevik Strand; and the Bjørndalen quarry, Tvedalen), at Kariåsen in the Sandefjord area, Norway, and in the Burpala alkaline complex, Baikal area, Russia.

PHYSICAL AND OPTICAL PROPERTIES

The type ferrokentbrooksite occurs as reddish brown to red, pseudo-octahedral crystals up to 1 cm in diameter (Fig. 1), although much larger crystals and masses have been found in other dykes at Mont Saint-Hilaire. Of the forms exhibited, $\{0001\}$, $\{10\bar{1}1\}$ and $\{01\bar{1}2\}$ are dominant, and $\{02\bar{2}1\}$ and $\{11\bar{2}0\}$ are minor. It is vitreous and transparent with a white streak. It is non-fluorescent in short and long-wave ultraviolet light. It is brittle, without cleavage or parting; it has an uneven to conchoidal fracture. It has a Mohs hardness of 5–6. The density of ferrokentbrooksite, measured by suspension in methylene iodide, is 3.06(3) g/cm^3, comparing well with the calculated density of 3.06 g/cm^3.

Ferrokentbrooksite is uniaxial negative, ω = 1.6221(3) and ε = 1.6186(3) (λ = 589 nm); some grains show an anomalous biaxial character, with $2V \approx 5°$. In transmitted light, thin grains exhibit a pale, rose-orange color. The mineral shows no pleochroism at maximum

Fig. 1. A crystal of ferrokentbrooksite 1.5 mm in diameter. W. Lane specimen. Photo by L. Horváth.

birefringence. A Gladstone–Dale calculation gives a compatibility index of 0.001, which is rated as superior (Mandarino 1981).

CHEMICAL COMPOSITION

Chemical analyses were done in wavelength-dispersion (WD) mode on a JEOL 733 electron microprobe using Tracor Northern 5500 and 5600 automation. Data reduction was done with a PAP routine in XMAQNT (pers. commun., C. Davidson, CSIRO). The accelerating voltage was 15 kV, and the beam current was 20 nA. Data for all elements in the samples were collected for 25 s or 0.50% precision, whichever was attained first. Forty-six elements were sought, but only those detected are reported here. The holotype specimen of ferrokentbrooksite displays very minor zoning using back-scattered electron imaging, and appears to be quite homogeneous in composition. The presence of H_2O was confirmed in ferrokentbrooksite by infrared spectroscopy and crystal-structure analysis. The following standards were used in the electron-microprobe analyses: albite (Na$K\alpha$), almandine (Si$K\alpha$, Fe$K\alpha$), vlasovite (Zr$L\alpha$), sanidine (K$K\alpha$), diopside (Ca$K\alpha$), rutile (Ti$K\alpha$), celestine (Sr$L\alpha$), tephroite (Mn$K\alpha$), chrysoberyl (Al$K\alpha$), a set of synthetic REE phosphates (La$L\alpha$, Ce$L\alpha$, Nd$L\alpha$, Sm$L\alpha$, Gd$L\alpha$), synthetic yttrium iron garnet (YIG) (Y$L\alpha$), synthetic hafnon (Hf$L\alpha$), synthetic MnNb$_2$O$_6$ (Nb$L\alpha$), synthetic NiTa$_2$O$_6$ (Ta$L\alpha$), phlogopite (F$K\alpha$) and marialite (Cl$K\alpha$). Data for elements in the standards were collected for 50 s or 0.25% precision, whichever was attained first. Eight chemical analyses were carried out on the holotype specimen of ferrokentbrooksite, two of which were performed on the grain on which the structure was performed. An average result of the latter two analyses is reported in Table 1 with the range given for all eight analyses. The amount of H_2O was calculated by stoichiometry from the crystal-structure analysis. The empirical formula of ferrokentbrooksite, based on 77.47 anions as determined in the crystal-structure analysis, is: $(Na_{13.05}REE_{0.99} K_{0.32}Ca_{0.23}Sr_{0.15})_{\Sigma14.74}(Ca_{4.59}Mn_{1.24}Y_{0.17})_{\Sigma6}(Fe_{2.39} Mn_{0.61})_{\Sigma3}(Zr_{3.00}Ti_{0.04}Hf_{0.03})_{\Sigma3.07}(Nb_{0.64}Si_{0.23}Zr_{0.07} Ta_{0.02})_{\Sigma0.96}(Si_{24.93}Al_{0.07})_{\Sigma25}O_{73}(O,OH,H_2O)_{\Sigma2.47}(Cl_{0.89} F_{0.71}OH_{0.40})_{\Sigma2}$ or, ideally, $Na_{15}Ca_6(Fe,Mn)_3Zr_3NbSi_{25} O_{73}(O,OH,H_2O)_3(Cl,F,OH)_2$.

TABLE 1. FERROKENTBROOKSITE: CHEMICAL COMPOSITION

|	wt.%	Range		wt.%	Range
Na$_2$O	11.96	11.93–12.56	SiO$_2$	44.70	44.53–45.65
K$_2$O	0.44	0.44–0.49	TiO$_2$	0.09	0.08–0.10
CaO	7.99	7.36–8.05	ZrO$_2$	11.20	11.12–11.64
MnO	3.88	3.37–4.00	HfO$_2$	0.17	0.12–0.20
FeO	5.08	5.01–5.46	Nb$_2$O$_5$	2.51	1.81–2.54
SrO	0.45	0.39–0.46	Ta$_2$O$_5$	0.16	0.09–0.21
Al$_2$O$_3$	0.11	0.10–0.20	F	0.40	0.00–0.42
Y$_2$O$_3$	0.58	0.47–0.61	Cl	0.93	0.86–0.96
La$_2$O$_3$	1.51	1.03–1.52	H$_2$O	0.35	
Ce$_2$O$_3$	2.51	1.77–2.54			
Nd$_2$O$_3$	0.53	0.43–0.79	O≡F,Cl	–0.38	
Sm$_2$O$_3$	0.11	0.00–0.23			
Gd$_2$O$_3$	0.17	0.00–0.19	Total	95.45	
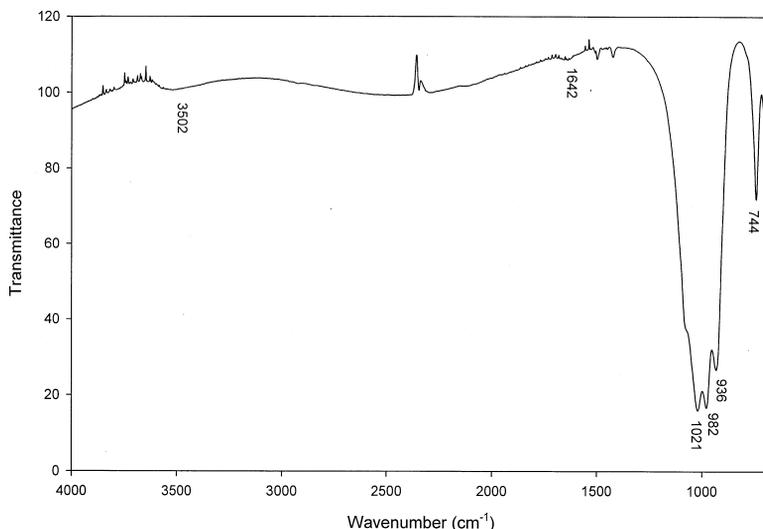
Fɪɢ. 2.   Infrared spectrum of ferrokentbrooksite.

INFRARED ANALYSIS

For analysis by Fourier transform infrared (FTIR) spectroscopy, a portion of the sample was positioned in a diamond anvil microsample cell and analyzed using a Spectra–Tech IR–Plan Research microscope interfaced to a Bomem Michelson MB–120 spectrometer. Two hundred scans were collected in the range 4000–660 cm^{-1} (Fig. 2). The broad absorption bands at approximately 3500 and 1650 cm^{-1} are assigned to the [OH] stretching mode and the [H$_2$O] bending mode, respectively. The two small bands at 1425 and 1500 cm^{-1} are attributed to the stretching mode of a [CO$_3$] group. The presence of (CO$_3$) in the eudialyte structure is discussed by Johnsen *et al*. (1999b). The bands at 940, 980, and 1020 cm^{-1} are assigned to the symmetric stretching of [SiO$_4$] and indicate considerable splitting of the [SiO$_4$] vibration modes, attributable to a structure with more than one crystallographically distinct [SiO$_4$] group. Bands at 700 and 745 cm^{-1} are assigned to bending of [SiO$_4$].

X-RAY CRYSTALLOGRAPHY
AND CRYSTAL-STRUCTURE DETERMINATION

X-ray powder-diffraction data collected on a Stoe transmission-type diffractometer are shown in Table 2. We used Cu$K\alpha_1$ radiation with a curved Ge monochromator. The data were collected in transmission-scan mode on a flat sample. Intensities were measured with a linear position-sensitive detector with an aperture covering a range of 6° in 2θ, step scan of 0.01°, and a 2θ range 5–90°; the total time of data collection was 65 h. Least-squares refinements based on 69 reflections gave the unit-cell parameters *a* 14.2099(7), *c* 30.067(2) Å. Full unit-cell data are given in Table 3.

The single crystal of ferrokentbrooksite used for the collection of X-ray diffraction intensity data is a ground sphere 0.17 mm in diameter. Intensity data were collected on a Siemens fully automated four-circle diffractometer operated at 50 kV and 40 mA with graphite-monochromated Mo$K\alpha$ radiation. A set of 42 reflections were used to center the crystal and refine the cell parameters. Assuming a non-centrosymmetric rhombohedral cell, one asymmetric unit of intensity data was collected (*i.e.,* $+ h + k \pm l$) to 2θ = 60° using a θ:2θ scan-mode, with scan speeds inversely proportional to intensity, varying from 4 to 29.3°/minute. Approximately 3800 reflections with more than 85% observed (*i.e.*, $F_o > 4\sigma F_o$) were collected. Information relevant to the data collection and structure determination is given in Table 4.

For the ellipsoidal absorption correction, 14 intense diffraction-maxima in the range 12 to 60° 2θ were chosen for Ψ diffraction-vector scans after the method of North *et al.* (1968). The converging *R* for the Ψ-scan data set decreased from 1.59% before the absorption correction to 1.07% after the absorption correction. The excellent converging *R*-values attest to the near-spherical shape of the crystals. Reduction of the intensity data, structure determination and initial refinement of the structure were done with the SHELXTL (Sheldrick 1990) package of computer programs. The final refinements were done with the SHELXL–93 program (Sheldrick 1993). The strategy applied to the final stages of the refinement is described in detail by Johnsen & Grice (1999).

The final coordinates and isotropic displacement parameters of the atoms in the ferrokentbrooksite structure were presented by Johnsen & Grice (1999, crystal #2). Lists of observed and calculated structure-factors, anisotropic displacement factors and selected bond-lengths have been submitted to the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario, K1A 0S2, Canada.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

Ferrokentbrooksite is a member of the eudialyte group. As described by Johnsen & Grice (1999), the structure of eudialyte-group minerals consists of layers of six-membered rings of $[M(1)O_6]$ octahedra (mainly Ca) joined by $[M(2)O_n]$ polyhedra (Fe or Mn) and sandwiched between two pseudocentrosymmetrically related layers of three-membered and nine-membered silicate rings forming a 2:1 composite layer. The 2:1 composite layers are cross-linked by Zr in octahedral coordination and are related to one another in accordance with the rhombohedral symmetry. Voids in the open structure are filled with five distinct $[Na\Phi_n]$ polyhedra, of which the $[Na(4)\Phi_n]$ polyhedron is particularly suitable as a host of relatively heavy elements such as REE and Sr. $M(3)$ and $Si(7)$ are two central sites of the two crystallographically distinct nine-membered silicate rings, and related

by the substitution $^{[6]}M(3) + {}^{[4]}Si(7) \Leftrightarrow 2^{[4]}Si(7)$, in which $M(3)$ typically is occupied by Nb.

The eudialyte structure is more or less centrosymmetric depending on the degree of disorder and the chemical content of certain sites. Eudialyte *sensu lato* rich in Si, Fe and Ca represent the most centrosymmetric structures. As substitutions of the type Si $\Rightarrow$ (Nb,W), Fe $\Rightarrow$ Mn, (Ca,Na) $\Rightarrow$ (REE,Sr) take place, the structures become progressively more non-centrosymmetric (Johnsen & Grice 1999). The expression of centrosymmetry is dependent on the composition within the solid-solution series between eudialyte *s.s.* (*Eud*) and kentbrooksite (*Ktb*) with an extension to oneillite, a *R3*-type eudialyte (Johnsen & Grice 1999, Johnsen *et al.* 1999b).

As a mineral species, ferrokentbrooksite is defined as the ferrous-iron-dominant analogue of kentbrooksite with Fe as the predominant element in $M(2)$ replacing Mn. Structurally, ferrokentbrooksite and kentbrooksite are alike in having the disordered $M(2)$ cation mostly in five-fold coordination as opposed to eudialyte *s.s.*, which has the $M(2)$ cation in four-fold coordination in an almost planar arrangement. Ferrokentbrooksite is among the relatively few eudialyte-group minerals with $M(2)$ [$M(2,4)$ and $M(2,5)$ together] close to being fully occupied. Bond-valence calculations indicate that the Fe in ferrokentbrooksite is divalent.

Ferrokentbrooksite is further characterized by being an intermediate member of the *Eud–Ktb* solid-solution series. It is "moderately acentric", with a $|E^2 - 1|$ value of 0.871 (Table 4), which is primarily associated with a

TABLE 2. FERROKENTBROOKSITE: POWDER-DIFFRACTION DATA

I/I_0	d_{obs}	d_{calc}	h	k	l	I/I_0	d_{obs}	d_{calc}	h	k	l
26	11.402	11.389	1	0	1	7	2.380	2.381	0	4	8
7	10.083	10.022	0	0	3	9	2.367	2.367	1	4	6
11	9.545	9.523	0	1	2	13	2.319	2.319	2	4	1
38	7.104	7.105	1	1	0	8	2.257	2.256	1	3	10
25	6.414	6.415	0	1	4	7	2.205	2.204	5	1	1
16	6.029	6.028	0	2	1	10	2.187	2.187	1	5	2
50	5.694	5.695	2	0	2	4	2.169	2.169	4	2	5
5	5.405	5.403	0	1	5	19	2.150	2.150	4	0	10
43	4.300	4.301	2	0	5	6	2.134	2.133	3	1	11
19	4.095	4.095	1	1	6	5	2.120	2.120	5	1	4
31	3.955	3.955	2	1	4	5	2.093	2.093	1	4	9
22	3.796	3.796	3	0	3	6	2.057	2.058	3	2	10
7	3.678	3.679	1	2	5	6	2.009	2.009	0	6	3
4	3.591	3.594	0	1	8	23	1.977	1.978	4	2	8
24	3.552	3.552	2	2	0	7	1.953	1.954	4	3	4
51	3.391	3.391	1	3	1	9	1.932	1.932	3	3	9
12	3.329	3.328	3	1	2	10	1.898	1.898	6	0	6
31	3.207	3.207	2	0	8	4	1.873	1.873	1	6	1
8	3.174	3.174	3	0	6	7	1.839	1.840	2	4	10
31	3.155	3.156	2	1	7	5	1.833	1.832	1	4	12
21	3.019	3.023	1	1	9	31	1.776	1.776	4	4	0
100	2.968	2.968	3	1	5	13	1.761	1.761	0	4	14
6	2.922	2.923	1	2	8	5	1.746	1.746	2	2	15
19	2.898	2.898	2	2	6	4	1.721	1.721	3	3	12
98	2.847	2.847	4	0	4	14	1.674	1.674	4	4	6
6	2.776	2.775	2	3	2	7	1.641	1.642	2	6	5
5	2.739	2.739	0	4	5	18	1.603	1.604	4	0	16
17	2.700	2.701	0	2	10	8	1.592	1.592	1	6	10
11	2.672	2.672	1	3	7	6	1.541	1.540	1	5	14
15	2.643	2.643	3	2	4	7	1.531	1.530	8	0	2
20	2.590	2.590	0	3	9	8	1.479	1.479	5	3	11
9	2.525	2.525	2	1	10	5	1.424	1.424	8	0	8
7	2.505	2.506	0	0	12	4	1.410	1.410	4	6	1
6	2.453	2.453	0	5	1	4	1.405	1.405	2	5	15
						6	1.401	1.401	1	8	5

Stoe diffractometer data, transmission mode on flat sample; Cu$K\alpha_1$ radiation. Reflections with $I/I_0 < 4$ not included. Indexing based on the trigonal cell: a 14.2099(7), c 30.067(2) Å, V 5257.7(3) Å^3. Values of d_{obs} and d_{calc} are expressed in Å.

TABLE 3. FERROKENTBROOKSITE: UNIT-CELL DATA

Crystal system	trigonal	Space group	R3m
a	14.2099(7) Å	c	30.067(2) Å
c:a	2.1159	V	5257.7(3) Å^3
Z	3		

TABLE 4. FERROKENTBROOKSITE: CRYSTAL DATA AND INFORMATION ON STRUCTURE REFINEMENT

Sample identification	ferrokentbrooksite (crystal #2 in Johnsen & Grice 1999)
Wavelength	0.71073 Å
Crystal system: space group	Trigonal: R3m
Unit-cell dimensions	a 14.2277(6), c 29.987(2) Å
Volume	5256.9(5) Å^3
Crystal size	sphere 0.17 mm in diameter
θ range for data collection	2.04 to 30.06°
Index ranges	$0 \le h \le 17$, $0 \le k \le 17$, $-42 \le l \le 42$
Reflections collected	3824
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3824 / 0 / 292
Goodness-of-fit on F^2	1.017
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.042$, $wR2 = 0.083$
R indices (all data)	$R1 = 0.055$, $wR2 = 0.089$
Isotropic refinement	$R1 / wR2$: 0.070 / 0.133
Largest diff. peak and hole	1.06 and -1.12 $e \cdot \text{Å}^{-3}$
Ψ convergence before/after	1.59 / 1.07
$|E^2 - 1|$	0.871

moderate content of Nb and other relatively heavy elements at $M(3)$, the coordination of $M(2)$ being predominantly five-fold, and a notable but moderate difference in scattering power between the two pseudocentrosymmetrically related sites $Na(3)$ and $Na(4)$ (Johnsen & Grice 1999, Fig. 11). A complete site-assignment of ferrokentbrooksite is presented by Johnsen & Grice (1999).

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