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FERROCHIAVENNITE, A NEW BERYLLIUM SILICATE ZEOLITE FROM SYENITE PEGMATITES IN THE LARVIK PLUTONIC COMPLEX, OSLO REGION, SOUTHERN NORWAY

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ABSTRACT

Ferrochiavennite is a new beryllium silicate zeolite with chemical composition close to $Ca_{1-2}FeSi_5Be_2O_{13}(OH)_2{\cdot}2H_2O$. It is described from two syenite pegmatite localities in Norway: Blåfjell, Langangen, Telemark, and the AS Granit larvikite quarry, Tvedalen, Vestfold. The mineral is monoclinic, $P2_1/c$, with a 8.759(5), b 4.864(2), c 31.258(6) Å, β 90.31(6)°, V 1331.7(6) Å^3, and $Z = 4$. The crystal structure was refined to $R_1 = 0.048$ for 3651 observed reflections. The zeolite structure is isostructural with chiavennite, consisting of intersecting channels of nine-, six-, five-, and four-fold rings. The strongest eight reflections of the X-ray powder-diffraction pattern [d(obs.) in Å (I) (hkl)] are: 15.555 (100) (002), 4.104 (29) ($\bar{1}12$, 112), 3.938 (36) ($\bar{1}13$, 113), 3.909 (60) (008), 3.820 (30) ($\bar{2}04$, 204), 3.251 (66) (017, 210, $\bar{2}11$), 3.186 (27) ($\bar{2}12$, 212), 2.884 (64) ($\bar{2}15$, 215). The mineral is biaxial (+) with refractive indices α 1.583(1), β 1.589(1), γ 1.602(1), measured at 590 nm. $2V$ (meas.) = 62(4)° from extinction curves $2V$ = 76(5)°; $2V$ (calc.) = 69°. The optical orientation is $X \sim a$, $Y \sim c$, and $Z \sim b$. The Mohs hardness is ~ 3; D(meas.) = 2.67(2) and D(calc.) = 2.709 g/cm^3.

Keywords: ferrochiavennite, new mineral species, zeolite, beryllium silicate, crystal structure, syenitic pegmatite, Norway

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INTRODUCTION

The Larvik Plutonic Complex (LPC) occupies the 50 km long and 20 km wide area between the Oslofjord in the east and the Langesundsfjord in the west and is the southern part of the Oslo rift, which was formed by intracontinental magmatic activity in late Carboniferous and early Permian time. The LPC, especially its western district, hosts a large number of pegmatites, some of which show a rich assemblage of rare and unique minerals. The mineralogy of these pegmatites became famous through the monograph by Brøgger (1890). Today about 200 different species have been identified (Larsen 2010).

The pegmatites in the LPC are unique in their extreme enrichment of late-stage beryllium minerals, mainly silicates, presumably derived from the hydrothermal breakdown of the primary Be-silicates leucophanite and meliphanite, and partly the Be-borate hambergite. The alteration and breakdown of other minerals which contain significant amounts of beryllium, such as aegirine, nepheline, and thorite (Raade 2008), may also be a source of beryllium. A total of 40 valid beryllium minerals are known from syenitic pegmatites or alkaline rocks (Raade 2008, Pekov *et al.* 2008, Grice *et al.* 2009, Raade *et al.* 2009), and 65% of them occur in Norway. Brøgger (1890) was the first to describe new beryllium minerals such as leucophanite, meliphanite, hambergite, and eudidymite. Today we know of at least 20 valid Be-silicates in addition to the two Be-borates hambergite and berborite (Giuseppetti *et al.* 1990) and the Be-hydroxides/oxides behoite, chrysoberyl, and bromellite (Larsen *et al.* 1987) from LPC syenitic pegmatites. Chiavennite, described as a new mineral by Raade *et al.* (1983), is currently known from at least 20 locations within the LPC.

No other alkaline complex in the world supersedes the number of beryllium minerals found in the Larvik complex; with 19 in the Ilímaussaq intrusion, Greenland (Petersen 2001), 16 in Mont St. Hilaire, Canada (Back *et al.* 2011), and 13 in the Khibiny massif, Kola peninsula, Russia (Men'shikov *et al.* 1999).

In this paper we present yet another new zeolitic Be-silicate from the LPC, the Fe-dominant analogue of chiavennite (Bondi *et al.* 1983, Raade *et al.* 1983). The mineral and name were approved by the Commission on New Minerals, Nomenclature and Classification (IMA No. 2012-039). Holotype material is preserved in the Canadian Museum of Nature, Ottawa, Canada, specimen number CMNMC 86554 and the Department of Geology, Natural History Museum, University of Oslo (catalogue number 42108).

OCCURRENCES

Ferrochiavennite was identified from two different localities, and work was carried out by two individual groups. As we learned of each other's work, it was decided to combine the description of the species from the two type localities. The Localities denoted 1 and 2 below are used throughout the paper to distinguish which locality the data refer to; if no specific locality is given, the data is for material from Locality 1.

Locality 1

The only sample of ferrochiavennite was collected by one of us (RK) in 1976 from a road-cut during the construction of the new highway E-18 between Larvik (Vestfold) and Porsgrunn (Telemark) at Blåfjell, Langangen, Telemark (59º5′34"N, 9º41′38"E). A handful of samples were collected from the ditch and the following magmatic minerals were identified: microcline, albite, annite, zircon, pyrochlore, fayalite, magnetite, and gadolinite-(Ce). Aegirine, pyrophanite, nepheline, calcite, analcime, natrolite, pyrite, molybdenite, galena, sphalerite, gugiaite, hambergite, ferrochiavennite, and chlorite are of hydrothermal origin. None of the samples were found *in situ*. The major part of the sample of ferrochiavennite is associated with albite, magnetite, and fayalite, with minor amounts of zircon, nepheline, analcime, pyrite, and hambergite.

Arne Åsheim, a private collector in Porsgrunn, discovered samples of the new mineral chiavennite in 1975 (Larsen & Åsheim 1976; Raade *et al.* 1983), approximately 100 m west of the locality for ferrochiavennite.

Locality 2

Samples containing a pale greenish chiavennite-like mineral were found in 2008 by the private collector-couple Jens Andreas and Tordis Larsen in waste rock on level 3 in the AS Granit larvikite quarry, Tvedalen, Vestfold (59º2′21"N, 9º51′25"E). The mineral was investigated by one of the authors (AOL) in 2010 and was subsequently identified as a Fe-dominant chiavennite. Chiavennite (*senso stricto*) is rather common in the AS Granit quarry and the neighboring Tuften quarry. The latter quarry is the type locality for another Be-zeolite, namely alflarsenite (Raade *et al.* 2009). Ferrochiavennite crystallized very late during the hydrothermal stage of the pegmatite formation. The mineral occurs in small vugs in masses of analcime associated with hambergite. Other late-stage minerals include tvedalite, apophyllite-(KF), natrolite, gonnardite, pale yellowish white chiavennite, epididymite, behoite, calcite, chlorite, aegirine, catapleiite, gaidonnayite, neotocite, fluorite, and molybdenite. Ferrochiavennite often occurs only in the rim of the spherules where tvedalite makes up the center, rather analogous to the occurrence of tvedalite at the type locality, where the tvedalite is covered by chiavennite (Larsen *et al.* 1992). The primary part of the pegmatite consists of a greyish microcline plus minor amounts of biotite, zircon, a britholite-like mineral, and pyrochlore.

PHYSICAL AND OPTICAL PROPERTIES

Crystal aggregates of ferrochiavennite form spherules up to ~ 2 mm in diameter (Locality 1). Individual crystals are about 0.2 × 0.2 × 0.02 mm, platy on {001} and spear shaped along [100]. Spherules (Locality 2) are up to 1 mm across, but individual crystals are significantly smaller than at locality 1. The spheres of ferrochiavennite at Blåfjell, Langangen are often coated with minute crystals of analcime (Fig. 1) and are beige or pale yellow (Fig. 2), while at Tvedalen it is very pale green. Streak is white and luster vitreous to translucent. The mineral is non-fluorescent in long- and short-wave ultraviolet. Mohs hardness ~ 3, brittle with an uneven fracture, and no cleavage was observed. The density (Blåfjell), measured by flotation in heavy liquids, is 2.67(2) g/cm^3, which compares reasonably with the calculated densities of 2.709 g/cm^3 (Locality 1) and 2.7209 g/cm^3 (Locality 2).

The optical properties (Blåfjell) measured in Na light (590 nm) are biaxial (+) with, $\alpha = 1.583(1)$, $\beta = 1.589(2)$, $\gamma = 1.602(1)$, $2V$ (meas. by extinction curves) = 62(4)°, $2V$ (calc.) = 69° , orientation: $X \approx a$, $Y \approx c$, $Z = b$. Ferrochiavennite is nonpleochroic and dispersion could not be determined.

CHEMICAL COMPOSITION

Chemical analyses were carried out in two separate laboratories. For the Blåfjell (Locality 1) material 10 analyses were done at the Canadian Museum of Nature by wavelength-dispersive electron-microprobe (EMP) at 15 kV, 20 nA, 10 μm beam diameter. Fluorine was below detection limits. H_2O was calculated by stoichiometry from the results of the crystal structure analysis (Hawthorne & Grice 1990); all H atoms were found. BeO was calculated by stoichiometry from the results of the crystal structure analysis.

For the Tvedalen material (Locality 2) seven analyses were done at the Department of Geosciences, University of Oslo using a Cameca SX100 electron-microprobe operated in WDS mode with a an acceleration voltage of 15 kV, a current of 6 nA, and a beam diameter of 10 μm. Intensity data were corrected for inter-element overlaps, and for matrix effects using a Cameca version of the 'PAP PhiRhoZ' program (Pouchou & Pichoir 1984).

Analytical data and calculated formulae based on 17 anions and seven tetrahedral sites are given in Table 1.

X-RAY CRYSTALLOGRAPHY

X-ray powder diffraction

Table 2 displays the X-ray powder-diffraction data of ferrochiavennite, obtained with a Bruker AXS Discover 8 micro-diffractometer using a Hi-Star 2-D area detector, Cu$K\alpha_1$ radiation, and calibrated using the method of Rowe (2009). Unit-cell parameters refined from the powder data for space group $P2_1/c$ are: a 8.759(5), b 4.864(2), c 31.258(6) Å, β 90.31(6)°, V 1331.7(6) Å^3, $Z = 4$.

Indexing powder diffraction data in a monoclinic cell that has pseudo-orthorhombic symmetry is problematic due to the resolution limits of a micro-diffractometer. In a monoclinic cell with β very close to 90°, the difference in 2θ values between diverging reflections is too small to be resolved by the micro-diffractometer and will combine into a single observed peak. This means that the monoclinic character of the structure will not be perceived in the powder data and will look just like a pattern of the equivalent orthorhombic cell. This is obvious in Table 2, in which many measured peaks have at least two contributing reflections with close d-spacings in the calculated pattern. For such cases the two or more unresolved reflections are not suitable for

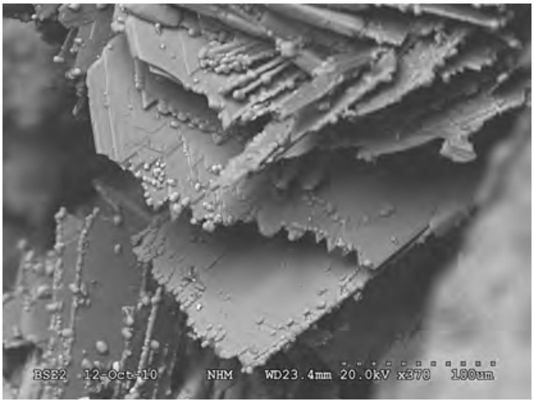

FIG. 1. SEM image of ferrochiavennite with small, adhering spheres of analcime from Blåfjell, Langangen, Norway.

FIG. 2. Ferrochiavennite, Blåfjell, Langangen, Norway. Field of view 2 mm. Photo: Roy Kristiansen.

TABLE 1. FERROCHIAVENNITE ANALYTICAL DATA

Constituent	wt.%	Range	SD	Probe Standard
		[1] Blåfjell (10 analyses)		
SiO_2	46.00	44.06−49.12	1.72	diopside
Al_2O_3	4.64	3.97−6.28	0.83	sanidine
FeO	5.29	3.64−6.99	1.16	hematite
MnO	4.04	2.60−5.06	0.81	tephroite
MgO	0.13	0.09−0.17	0.03	diopside
CaO	17.62	10.50−24.32	4.23	diopside
Na_2O	0.73	0.50−0.86	0.20	albite
K_2O	0.02	0.01−0.03	0.01	sanidine
BeO	10.37			
H_2O	9.81			
Total	98.65			
		[2] A/S Granit (7 analyses)		
SiO_2	46.41	42.82–48.76	2.12	wollastonite
Al_2O_3	2.76	1.83–3.78	0.82	Al_2O_3
FeO	9.94	8.25–10.83	0.91	Metal
MnO	3.53	2.33–4.93	0.83	pyrophanite
CaO	12.23	10.94–14.56	1.29	wollastonite
Na_2O	1.00	0.58–1.68	0.42	albite
K_2O	0.02	0.01–0.04	0.01	orthoclase
BeO	9.91			
H_2O	9.44			
Total	95.24			

The empirical formulae (based on 17 anions *pfu* and 7 tetrahedral framework sites) are as follows:
[1]: $(Ca_{1.73}Na_{0.13})_{\Sigma 1.86}(Fe_{0.41}Mn_{0.31}Mg_{0.02})_{\Sigma 0.74}(Si_{4.22}Al_{0.50}Be_{2.28})_{\Sigma 7.00}O_{13}(OH)_2\cdot 2H_2O$
[2]: $(Ca_{1.25}Na_{0.19}Mn_{0.08})_{\Sigma 1.52}(Fe_{0.79}Mn_{0.21})_{\Sigma 1.00}(Si_{4.42}Al_{0.31}Be_{2.27})_{\Sigma 7.00}O_{13}(OH)_2\cdot 2H_2O$
The simplified formula is $Ca_{1-2}Fe[(Si,Al,Be)_5Be_2O_{13}(OH)_2]\cdot 2H_2O$.
The formula derived from the crystal structure refinement is $Ca_{1.16}Fe_{0.92}[(Si_{4.74}Be_{0.26})Be_2O_{13}(OH)_2]\cdot 2H_2O$.

indexing purposes. This ambiguity directly impacts on cell-refinement calculations with an increase in standard deviations.

Crystal structure analysis

The single crystal of ferrochiavennite [from the Blåfjell locality (Locality 1)] was a blade measuring 10 × 30 × 40 μm. Intensity data were collected with a Bruker D8 three circle diffractometer equipped with a rotating anode generator, multi-layer optics and an APEX-II CCD detector and operated at 50 kV, 24 mA. This setup yields a very intense X-ray beam. A full sphere of intensity data was collected up to $2\theta = 60°$ using 10 s frames with frame widths of 0.2°. Data pertinent to the intensity-data collection are given in Table 3. The unit-cell parameters for the single crystal were refined using 5523 indexed reflections. The mineral has a marked pseudo-orthorhombic cell which was used in the original structure determination of chiavennite described from Italy (Tazzoli *et al.* 1995). As there was a small, but significant, change from an orthonormal cell, ferrochiavennite was collected on a monoclinic cell. Attempts to find suitable single crystal material on the material from AS Granit all failed because of smaller, intergrown spherules of crystals compared to the Blåfjell locality and often not being able to separate the ferrochiavennite from the tvedalite.

The three-dimensional data were corrected for Lorentz, polarization, and background effects, and multiple-measured reflections were averaged using the Bruker program SAINT. An empirical absorption-correction was applied (SADABS, Sheldrick 1998). All calculations were done with the Siemens SHELXTL 5.1 suite of programs (Sheldrick 1997), with scattering factors of neutral atoms taken from the International Tables for X-ray Crystallography (Ibers & Hamilton 1974). The twinned crystal required the newer programs of Sheldrick (2008a, 2008b), CELL_ NOW and TWINABS, as the twin law, reflection on {100}, is not a merohedral twin, thus requiring individual data sets for each domain. Extinction conditions yielded $P2_1/c$ as the most probable space group. This space group, transformed to the setting of Tazzoli *et al.* (1995) is $P112_1/b$ (SG 14), a subgroup of their structure space group $P2_1/n2/a2_1/b$ or *Pnab* (SG 60). The twin by reflection on {100} partitions the domains into the proportion 0.63:0.37, and the refined value is 0.371(2). Tazzoli *et al*. (1995) noted exceptions to the extinction conditions for their chosen space group. With the present data set in space group *Pnab* the *R*(int) is 0.055 with 484 systematic absence violations and the final *R* for 1965 observed reflections is 0.105. Exception to the extinction conditions is definitely a warning sign

TABLE 2. FERROCHIAVENNITE: X-RAY POWDER DIFFRACTION DATA

I obs	*I* calc*	*d* obs	*d* calc**	*hkl*	*I* obs	*I* calc*	*d* obs	*d* calc**	*hkl*
100	100	**15.555**	15.629	002	12	8	2.380	2.380	$\bar{2}19$
24	20	7.766	7.814	004	15	8	2.322	2.322	024
24	12	5.813	5.847	$\bar{1}04$	9	3	2.254	2.260	$\bar{3}16$
	11		5.815	104		2		2.259	$\bar{2}.1.10$
10	4	4.806	4.806	011		3		2.252	316
9	2	4.395	4.407	013		2		2.250	2.1.10
	4		4.380	200	7	4	2.218	2.224	$\bar{1}.1.12$
29	9	**4.104**	4.106	$\bar{1}12$		3		2.219	1.1.12
	11		4.100	112	9	3	2.161	2.170	$\bar{4}02$
36	15	**3.938**	3.941	$\bar{1}13$		2		2.167	402
	9		3.933	113		3		2.166	$\bar{1}.0.14$
60	43	**3.909**	3.907	008		2		2.160	1.0.14
30	12	**3.820**	3.829	$\bar{2}04$		5		2.155	0.1.13
	10		3.812	204	9	4	1.9676	1.9703	$\bar{2}26$
66	4	**3.251**	3.289	017		4		1.9667	226
	37		3.255	210	12	2	1.9203	1.9376	$\bar{2}.1.13$
	8		3.238	$\bar{2}11$		4		1.9302	2.1.13
27	7	**3.186**	3.189	$\bar{2}12$		6		1.9194	0.2.10
	10		3.184	212	7	1	1.8677	1.8693	1.1.15
21	10	3.105	3.110	$\bar{2}13$		1		1.8654	228
	5		3.103	213	11	7	1.7775	1.7776	0.2.12
10	5	2.940	2.949	$\bar{1}.0.10$	13	7	1.6274	1.6273	420
	5		2.939	1.0.10	6	4	1.6038	1.6036	$\bar{2}.1.17$
64	20	**2.884**	2.892	$\bar{2}15$		2		1.5981	2.1.17
	31		2.882	215	5	2	1.5026	1.5044	$\bar{4}28$
12	10	2.823	2.826	019		2		1.5041	233
6	3	2.688	2.693	$\bar{1}19$		2		1.5001	428
	3		2.686	119	5	2	1.4938	1.4929	$\bar{2}34$
15	5	2.625	2.635	$\bar{2}17$		2		1.4919	234
	10		2.625	217		2		1.4780	$\bar{2}35$
8	3	2.505	2.522	$\bar{1}.1.10$					
	3		2.515	1.1.10					
	2		2.506	$\bar{2}18$					
	2		2.496	218					
	2		2.494	311					

*Calculated from the crystal structure determination.
**Calculated from XRPD cell refinement with *a* = 8.759(5), *b* = 4.864(2), *c* = 31.258(7) Å, β = 90.31(3)°.
Bold face type indicates the 8 strongest lines

TABLE 3 . FERROCHIAVENNITE: DATA COLLECTION AND STRUCTURE REFINEMENT INFORMATION

Space Group	$P2_1/c$ (No. 14)	Measured reflections	15716
a (Å)	8.7499(5)	Unique reflections	3956
b (Å)	4.9160(3)	Observed reflections [> 4σ(*F*)]	3651
c (Å)	31.431(2)	*R*(int) (%)	0.02
β (°)	90.1574(9)	Goodness of fit on F^2	1.21
V (Å^3)	1352.0(3)	*R* index for all data	0.051
μ (mm^{-1})	2.63	*R* index for observed data	0.048
Ideal unit-cell contents 4[$Ca_{1-2}Fe(Si_5Be_2O_{13}OH_2)\cdot 2H_2O$]			

that the space group symmetry is incorrect. For the structure solution the atomic positional parameters of Tazzoli *et al.* (1995) were transformed into the present cell. The atomic site labels of Tazzoli *et al.* (1995) were maintained and the sites generated by the change in symmetry are designated by a double digit, *e.g.*, Si2 is the original and Si22 is the new monoclinic symmetry-generated site. In this way readers may easily compare the two structures.

The H atoms were refined with a fixed isotropic displacement factor but with no constraints on the O–H distance. The addition of an isotropic extinction-correction did improve the refinement, attesting to the perfection of the crystal. The maximum and minimum electron-densities in the final cycle of refinement were +0.82 and –1.00 $e^-/Å^3$. With all atoms located and assigning anisotropic displacement factors to all non-hydrogen atoms, the structure refined to $R = 0.048$.

The final positional and anisotropic displacement parameters of atoms are given in Table 4a and 4b and selected bond-lengths in Table 5. Tables listing the observed and calculated structure-factors may be

TABLE 4a. FERROCHIAVENITE: COORDINATES AND ISOTROPIC DISPLACEMENT PARAMETERS

Atom	*x/a*	*y/b*	*z/c*	$U_{eq.}$	sof
Fe1	½	½	0	0.0115(2)	0.930(3)
Fe2	0	½	0	0.0110(2)	0.904(3)
Ca1	0.7495(1)	0.4996(2)	–0.08735(2)	0.0149(1)	1
Ca2	0.789(3)	0.409(7)	0.8019(7)	0.062(4)	0.05
Ca22	0.7309(16)	0.491(4)	0.7998(3)	0.062(4)	0.111(4)
Si1	0.7501(2)	0.0004(2)	–0.00143(2)	0.0080(2)	0.951(3)
Be1	0.7501(2)	0.0004(2)	–0.00143(2)	0.0080(2)	0.049
Si2	0.4147(1)	0.5925(2)	–0.23247(3)	0.0105(2)	0.923(3)
Be2	0.4147(1)	0.5925(2)	–0.23247(3)	0.0105(2)	0.077
Si22	0.0832(1)	0.3662(2)	–0.23206(3)	0.0122(2)	0.944(4)
Be22	0.0832(1)	0.3662(2)	–0.23206(3)	0.0122(2)	0.056
Si3	0.1401(1)	0.2353(2)	–0.13453(3)	0.0098(2)	0.961(3)
Be3	0.1401(1)	0.2353(2)	–0.13453(3)	0.0098(2)	0.039
Si33	0.3552(1)	0.7230(2)	–0.13537(3)	0.0104(2)	0.957(3)
Be33	0.3552(1)	0.7230(2)	–0.13537(3)	0.0104(2)	0.043
Be4	0.5005(6)	0.0696(9)	0.05727(13)	0.0126(9)	1
Be44	0.0008(5)	0.9206(9)	0.05699(14)	0.0106(8)	1
O1	0.6522(3)	–0.2036(5)	–0.03284(7)	0.0111(5)	1
O2	0.8461(3)	0.2062(5)	–0.03221(8)	0.0140(5)	1
O3	0.8610(3)	–0.1867(5)	0.02756(8)	0.0118(5)	1
O4	0.6404(3)	0.1889(5)	0.02808(8)	0.0142(5)	1
O5	0.2495(5)	0.4782(8)	–0.24802(7)	0.0281(6)	1
O6	0.4551(4)	0.8514(7)	–0.26271(11)	0.0301(8)	1
O7	0.4162(4)	0.6810(8)	–0.18255(9)	0.0347(9)	1
O8	0.0502(4)	0.0832(7)	–0.25742(13)	0.0373(9)	1
O9	0.0795(4)	0.3200(8)	–0.18140(10)	0.0308(8)	1
O10	0.0029(3)	0.7779(6)	0.10341(8)	0.0154(5)	1
O11	0.2175(4)	0.9423(9)	–0.13682(13)	0.0476(10)	1
O12	0.2725(4)	0.4446(7)	–0.11893(9)	0.0304(8)	1
O13	0.4951(4)	0.8029(6)	–0.10544(8)	0.0180(6)	1
OH14	0.4910(3)	0.7412(5)	0.05822(8)	0.0135(5)	1
OH15	0.0184(3)	0.2548(6)	0.05819(9)	0.0174(6)	1
OW16	0.8402(5)	0.7450(7)	–0.14989(11)	0.0381(10)	1
OW17	0.6561(4)	0.2231(7)	–0.14540(10)	0.0259(7)	1
H14	0.556(7)	0.697(14)	0.070(2)	0.050*	1
H15	–0.050(8)	0.313(15)	0.072(2)	0.050*	1
H161	0.788(7)	0.776(15)	–0.139(2)	0.050*	1
H162	0.845(7)	0.721(14)	–0.177(2)	0.050*	1
H171	0.557(7)	0.273(14)	–0.166(2)	0.050*	1
H172	0.614(7)	0.072(14)	–0.141(2)	0.050*	1

*fixed *U*

TABLE 4b. FERROCHIAVENITE: ANISOTROPIC DISPLACEMENT PARAMETERS

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Fe1	0.0162(3)	0.0082(3)	0.0102(3)	–0.0003(2)	0.0022(3)	–0.0024(3)	0.0115(2)
Fe2	0.0167(4)	0.0066(3)	0.0096(3)	–0.0015(2)	–0.0019(3)	–0.0041(3)	0.0109(2)
Ca1	0.0201(2)	0.0116(2)	0.0129(2)	–0.0002(3)	0.0010(4)	–0.0018(2)	0.0149(1)
Ca2	0.053(6)	0.100(9)	0.032(3)	–0.004(5)	–0.024(5)	–0.031(6)	0.062(4)
Si1	0.0092(3)	0.0071(3)	0.0077(3)	0.0001(3)	0.0010(6)	–0.0034(3)	0.0080(2)
Si2	0.0112(4)	0.0115(4)	0.0089(4)	–0.0011(3)	0.0044(4)	–0.0031(3)	0.0105(2)
Si22	0.0169(5)	0.0089(4)	0.0108(4)	0.0018(3)	–0.0016(4)	–0.0011(4)	0.0122(2)
Si3	0.0083(4)	0.0115(4)	0.0097(4)	–0.0006(3)	–0.0010(3)	0.0024(3)	0.0098(2)
Si33	0.0152(4)	0.0092(4)	0.0069(4)	–0.0012(3)	–0.0005(4)	–0.0010(4)	0.0104(2)
Be4	0.020(2)	0.008(2)	0.010(2)	–0.003(1)	–0.000(2)	–0.009(2)	0.0126(9)
Be44	0.007(2)	0.011(2)	0.013(2)	0.000(2)	–0.003(2)	0.003(2)	0.0106(8)
O1	0.0068(9)	0.015(1)	0.011(1)	–0.0029(9)	–0.0044(8)	0.0022(9)	0.0111(5)
O2	0.020(1)	0.010(1)	0.012(1)	0.0036(9)	–0.003(1)	–0.003(1)	0.0140(6)
O3	0.0082(9)	0.016(1)	0.011(1)	0.0028(9)	0.0033(9)	–0.0015(9)	0.0118(5)
O4	0.019(1)	0.009(1)	0.014(1)	–0.0016(9)	0.007(1)	–0.002(1)	0.0142(5)
O5	0.030(1)	0.034(1)	0.021(1)	–0.005(1)	–0.005(2)	–0.009(1)	0.0281(6)
O6	0.031(2)	0.022(1)	0.0374(2)	0.00636	–0.000(1)	–0.008(1)	0.0301(8)
O7	0.0321(2)	0.061(2)	0.011(1)	–0.012(1)	0.002(1)	–0.007(2)	0.0347(9)
O8	0.026(2)	0.030(2)	0.056(2)	–0.016(2)	–0.008(2)	–0.013(1)	0.0373(9)
O9	0.020(1)	0.056(2)	0.016(1)	0.012(1)	–0.002(1)	–0.011(1)	0.0308(8)
O10	0.013(1)	0.021(1)	0.012(1)	0.0071(9)	0.0025(9)	–0.001(1)	0.0154(6)
O11	0.0233(2)	0.054(2)	0.065(2)	–0.01942	–0.010(1)	0.023(2)	0.047(1)
O12	0.027(2)	0.035(2)	0.029(1)	0.011(1)	–0.010(1)	–0.015(1)	0.0304(8)
O13	0.024(1)	0.023(1)	0.008(1)	–0.003(1)	0.003(1)	–0.010(1)	0.0180(6)
OH14	0.015(1)	0.009(1)	0.016(1)	0.0026(9)	–0.001(1)	–0.002(1)	0.0134(5)
OH15	0.019(1)	0.018(1)	0.014(1)	–0.004(1)	0.007(1)	–0.003(1)	0.0174(6)
OW16	0.061(2)	0.027(2)	0.027(2)	0.007(1)	0.009(2)	–0.001(2)	0.038(1)
OW17	0.026(1)	0.030(2)	0.022(1)	–0.00341	–0.007(1)	–0.006(1)	0.0259(7)

obtained from the Depository of Unpublished Data, on the MAC website [ferrochiavennite CM51_285].

DESCRIPTION OF THE STRUCTURE

Ferrochiavennite has an interrupted zeolite structure which is essentially isostructural with chiavennite (–CHI) (Baerlocher *et al.* 2007). The structure consists of cross-connecting channels of nine-, six-, five-, and four-fold rings. The nine-fold ring channel contains the Ca atoms and H_2O groups; the six- and five-fold channels are empty, and the four-fold channels contain the Fe atoms. The Fe-site has octahedral coordination. The two Ca sites differ. The fully occupied Ca1 site has eight-fold coordination with four O atoms, two OH groups, and two H_2O groups. The partially occupied and split Ca2/Ca22 site has six-fold coordination with four O atoms and the two H_2O groups. For this split site some of the bond distances are unrealistically short. The splitting of the site compensates for this problem in terms of the O atoms. For example, when Ca2–O6 = 2.49 Å, Ca22–O6 = 2.13 Å and so for all four O atoms, when one distance is too short the other is reasonable. But for both Ca2 and Ca22 the two H_2O groups are a bit too close. It is likely that if the Ca2/Ca22 site was fully occupied there would be room for only one H_2O group. The increase in positive charges would be counterbalanced by a shift in the Be:Si ratio. In the tetrahedral framework there are seven tetrahedral sites, five that are dominantly Si while the remaining two are Be. Beryllium tends to segregate in a beryllosilicate structure such that the Be atoms avoid adjacent sites. This phenomenon is explained by Grice (2010) in terms of bond-valence considerations. Beryllium tetrahedra are in ribbons parallel to the **a**-axis (Fig. 3). The interruption in the tetrahedral framework can be clearly seen in Figure 4. Each of the two Be tetrahedra have an apical OH group that terminates polymerization in to the channel. In the channel the H_2O groups H-bond to each other and to O atoms in the periphery of the channel (Fig. 5).

Coordination sequences, for all subtended angles, and vertex symbols, to ten shells, for each tetrahedral site are given in Table 6. Coordination sequences are identical for tetrahedral sites that are related by the orthorhombic pseudo-symmetry; *i.e.*, Si2/Si22, Si3/Si33, and Be4/Be44.The topological density (TD) is lower for Be sites than for Si sites; Grice (2010) explains this effect in detail. Similarly, the vertex symbols are identical for pseudo-symmetry related

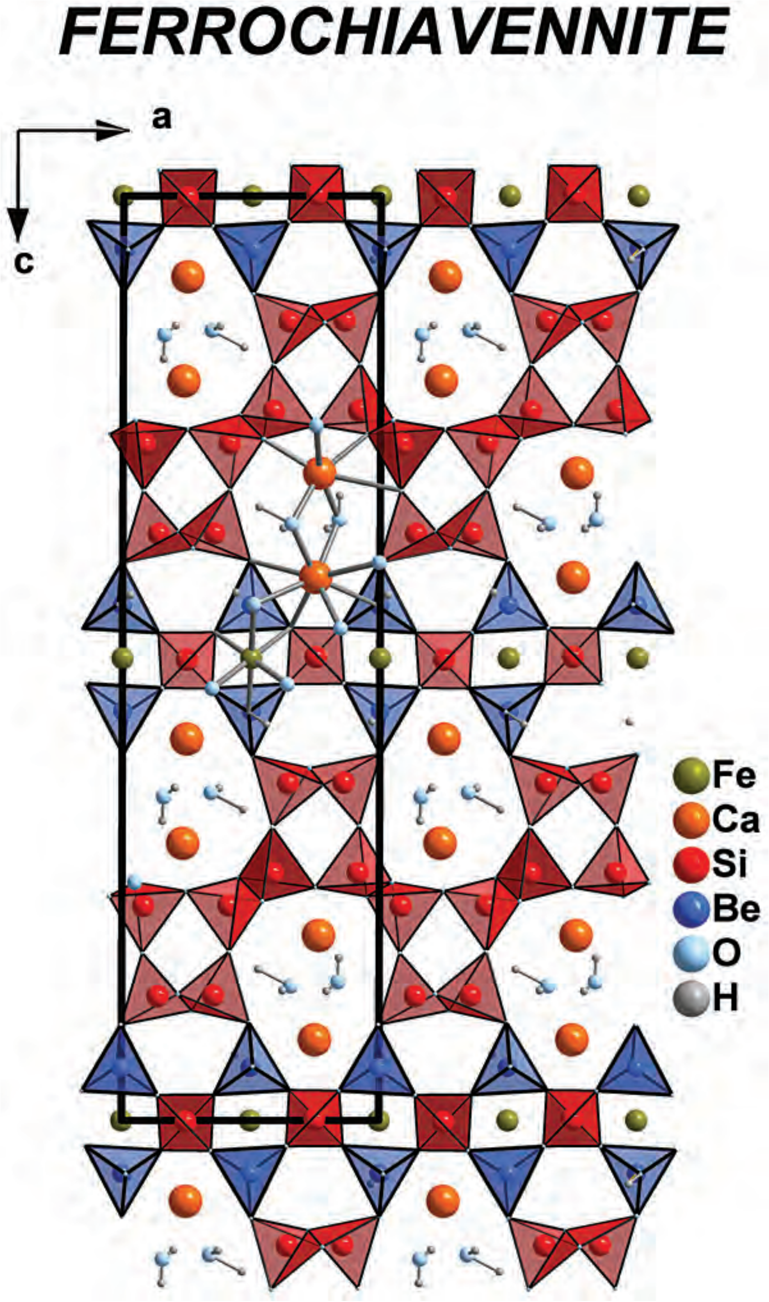

FIG. 3. Ferrochiavennite: a [010] projection showing the framework of tetrahedral polyhedra. The Ca atoms and H_2O groups (medium sized blue circles with H atoms) are centered in the nine-fold ring channels.

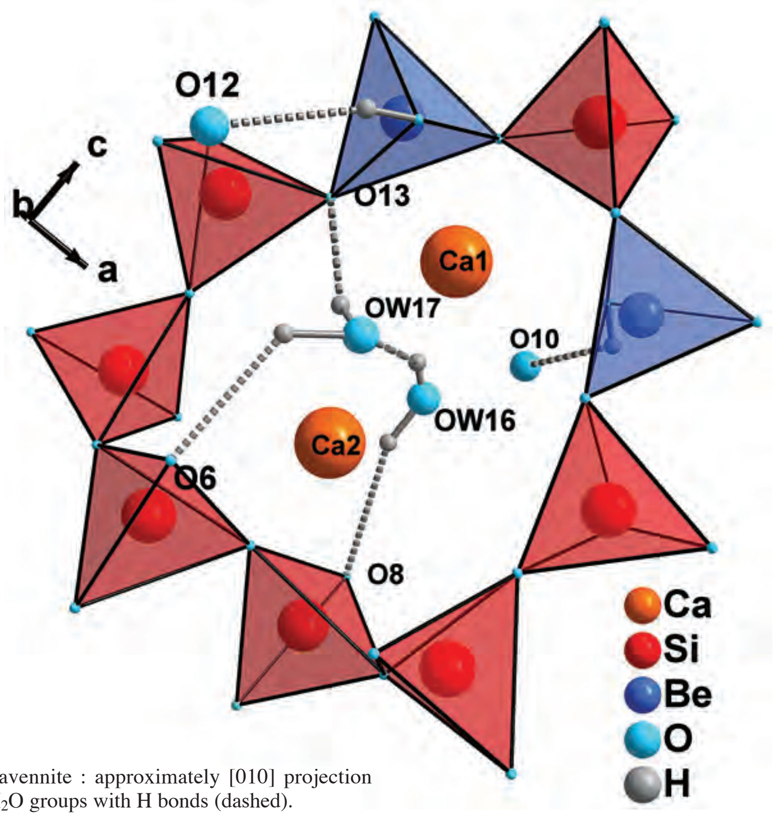

FIG. 4. Ferrochiavennite : approximately [010] projection showing the H_2O groups with H bonds (dashed).

FIG. 5. Ferrochiavennite : a [100] projection showing the OH groups that interrupt the polymerization of Be tetrahedra in one direction.

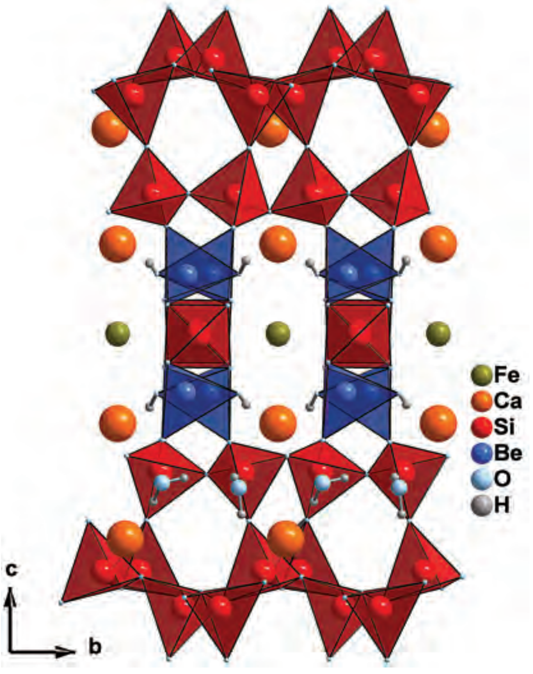

TABLE 5. FERROCHIAVENNITE: SELECTED BOND-LENGTHS (Å)

Fe1–O4	2.148(3) × 2	Fe2–O3	2.148(2) × 2		
Fe1–OH14	2.183(2) × 2	Fe2–OH15	2.195(2) × 2		
Fe1–O1	2.228(2) × 2	Fe2–O2	2.219(2) × 2		
<Fe1–O>	<2.186>	<Fe2–O>	<2.187>		
Ca1–O2	2.401(3)	Ca2–Ca22	0.66(4)	Ca22–Ca2	0.66(4)
Ca1–O1	2.409(3)	Ca2–O8	2.18(3)	Ca22–O6	2.13(1)
Ca1–OW17	2.417(3)	Ca2–OW17	2.21(3)	Ca22–OW16	2.22(1)
Ca1–OW16	2.438(4)	Ca2–OW16	2.30(3)	Ca22–OW17	2.27(1)
Ca1–OH15	2.532(3)	Ca2–O6	2.49(2)	Ca22–O8	2.36(1)
Ca1–OH14	2.585(3)	Ca2–O9	2.62(3)	Ca22–O5	2.90(2)
Ca1–O10	2.610(3)	Ca2–O5	2.71(3)	Ca22–O7	2.98(2)
Ca1–O13	2.741(3)	<Ca2–O>	<2.418>	<Ca22–O>	<2.477>
<Ca1–O>	<2.517>				
Si1–O3	1.615(3)	Si2–O5	1.626(4)	Si22–O9	1.609(3)
Si1–O4	1.628(3)	Si2–O7	1.629(3)	Si22–O8	1.614(3)
Si1–O2	1.632(3)	Si2–O6	1.629(3)	Si22–O8	1.628(3)
Si1–O1	1.648(3)	Si2–O6	1.652(3)	Si22–O5	1.634(5)
<Si1–O>	<1.631>	<Si2–O>	<1.634>	<Si22–O>	<1.621>
Si3–O11	1.593(4)	Si33–O13	1.588(3)		
Si3–O10	1.593(3)	Si33–O7	1.589(3)		
Si3–O9	1.620(3)	Si33–O11	1.619(4)		
Si3–O12	1.622(3)	Si33–O12	1.634(3)		
<Si3–O>	<1.607>	<Si33–O>	<1.608>		
Be4–OH14	1.617(5)	Be44–O10	1.617(5)		
Be4–O4	1.639(5)	Be44–O3	1.621(5)		
Be4–O13	1.642(5)	Be44–OH15	1.650(5)		
Be4–O1	1.669(6)	Be44–O2	1.677(5)		
<Be4–O>	<1.642>	<Be44–O>	<1.641>		
D–H	d(D–H)	d(H•••A)	d(D•••A)	<DHA	A
OH14–H14	0.78(6)	2.20(6)	2.955(4)	164(6)	O12
OH15–H15	0.73(7)	2.55(7)	2.943(4)	116(6)	O10
OW16–H161	0.59(6)	2.48(7)	2.852(5)	123(8)	OW17
OW16–H162	0.86(6)	2.37(6)	3.175(5)	156(6)	O8
OW17–H171	1.10(6)	2.27(7)	3.107(5)	131(4)	O6
OW17–H172	0.85(7)	2.01(7)	2.800(4)	155(6)	O13

TABLE 6. FERROCHIAVENNITE: COORDINATION SEQUENCES AND VERTEX SYMBOLS

Tetrahedral site	Coordination Sequence	TD_{10}	Vertex symbol
Si1	4 6 14 28 56 80 114 152 190 236	880	4•4•5•9•10•10
Si2	4 11 22 40 64 89 120 160 203 248	961	$4\bullet6_3\bullet6\bullet6\bullet6_2\bullet6_2$
Si22	4 11 22 40 64 89 120 160 203 248	961	$4\bullet6_3\bullet6\bullet6\bullet6_2\bullet6_2$
Si3	4 10 20 36 60 86 115 157 196 238	922	$4\bullet5\bullet6\bullet6_3\bullet10_2$
Si33	4 10 20 36 60 86 115 157 196 238	922	$4\bullet5\bullet6\bullet6_3\bullet10_2$
Be4	3 8 13 29 53 80 113 147 193 231	870	4•5•9
Be44	3 8 13 29 53 80 113 147 193 231	870	4•5•9

sites. Because the Be sites are interrupted in the polymerization scheme they have a very short, and quite different, vertex symbol. The Si1 site, surrounded by Be tetrahedral sites, has a TD and vertex symbol more similar to Be than the other Si sites. Framework density (FD) is the number of tetrahedral sites in 1000 Å^3. For ferrochiavennite the FD = 20.0 tetrahedra/1000 Å^3. In Baerlocher *et al*. (2007) the maximum observed FD for a zeolite is 20.7 and they list five, all synthetic, over 20. Alflarsenite (Grice *et al*. 2010) is a mineral example of a zeolite with a slightly higher FD of 21.7/1000 Å^3.

Differences between the present structure description and that of Tazzoli *et al*. (1995) are: (1) change in crystal system from orthorhombic to monoclinic, (2) presence of a twin law, (3) Fe is dominant in the octahedral site *versus* Mn, (4) there are two Ca sites, one only partially filled, *versus* 1 Ca site in the Italian occurrence, and (5) all H sites were determined.

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