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LEONARDSENITE, $MgAlF_5(H_2O)_2$, A NEW MINERAL SPECIES FROM ELDFELL VOLCANO, HEIMAEY ISLAND, ICELAND

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Abstract

Leonardsenite (IMA2011-059), with ideal formula $MgAlF_5(H_2O)_2$, is a new fumarole mineral from Eldfell volcano, Iceland. It has also been found in volcanic encrustations from the Hekla crater, Iceland. The mineral forms a soft and friable mass of white crystals up to 20 μm in length. The streak is white and the luster is earthy. The calculated density is 2.31 g cm^{-3}. Leonardsenite is orthorhombic, space group *Imma*; the lattice parameters, obtained from Rietveld refinement of the XRPD data, are: *a* 7.055(1) Å, *b* 10.117(2) Å, *c* 6.813(1) Å, *V* 486.3(1) Å^3, and $Z = 4$. The eight strongest reflections in the X-ray powder diffraction pattern are [*d* in Å (*I*) (*hkl*)]: 5.66 (100) (011), 4.92 (29) (101), 3.53 (27) (200), 3.03 (31) (031), 3.00 (38) (211), 2.30 (16) (231), 1.77 (19) (400), 1.76 (24) (242). Chemical analyses by energy-dispersive spectrometry using a scanning electron microscope produced a mean elemental composition as follows (wt.%): Mg 14.66, Al 16.16, F 52.98, O 15.88, H 1.78, total 101.46. The corresponding empirical formula, calculated on the basis of 2 cations *pfu*, is $Mg_{1.00}Al_{1.00}[F_{4.64}(OH)_{0.36}]_{\Sigma 5.00}(H_2O)_{1.29}$. On the basis of chemical analyses and X-ray diffraction data, leonardsenite corresponds to the synthetic compound $MgAlF_5(H_2O)_2$. The crystal structure of leonardsenite contains infinite chains of $[AlF_6]$ octahedra along the *c*-axis which are connected *via* common fluorine atoms to isolated $[MgF_4(H_2O)_2]$ octahedra. Leonardsenite is the first aluminum fluoride hydrated mineral of the inverse weberite group with general formula $M^{II}M^{III}F_5(H_2O)_2$. Leonardsenite belongs to the group of fluorides with interesting optical and catalytic properties. The name of this new species honors Erik Leonardsen (1934–), the former leader of the X-Ray Diffraction Laboratory of the Geological Institute, University of Copenhagen. The mineral and its name have been approved by the IMA-CNMNC (IMA2011-059).

Keywords: leonardsenite, new mineral, sublimates, fumaroles, fluoride, crystal structure, Eldfell, Hekla, Iceland

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INTRODUCTION

Leonardsenite was initially found in a post-eruptional encrustation collected in 1988 at Eldfell volcano, Iceland, subsequent to the 1973 eruption (Thorarinsson *et al.* 1973, Jakobsson *et al.* 1973). Successive investigations led to the discovery of leonardsenite in fumarole encrustations deposited at the Hekla crater subsequent to the 1991 eruption (Gudmundsson *et al.* 1992).

At the time the samples were collected, Eldfell and Hekla volcanoes (Fig. 1) were characterized by medium to low temperature fumaroles and by a very rich mineralogy characterized mainly by sulfates, fluorides, and fluorosilicates (Oskarsson 1981, Jakobsson *et al.* 2008, Balić-Žunić *et al.* 2009, 2010, 2012, Garavelli *et al.* 2009, 2010a, 2010b, Mitolo *et al.* 2008, 2010).

The following phases from the above localities, listed by Smith & Nickel (2007) as valid unnamed minerals, were reported by Jakobsson *et al.* (2008): $Na_2Ca_3Al_2F_{14}$ (UM2008-26-F:AlCaNa), $AlF_3•3H_2O$ (UM2008-27-F:AlHO), $NH_4(Fe,Co)_2F_6$ (UM2008-29F:CoFeHN), $FeF_3•3H_2O$ (UM2008-30-F:FeHO), $FeSiF_6•6H_2O$ (UM2008-31-F:FeHOSi), and $Na_3Fe(SO_4)_3$ (UM2008-49-SO:FeNa). More detailed investigations led to the approval, to date, of four new minerals: eldfellite, $NaFe(SO_4)_2$ (Balić-Žunić *et al.* 2009); heklaite, $KNaSiF_6$ (Garavelli *et al.* 2010a); jakobssonite, $CaAlF_5$ (Balić-Žunić *et al.* 2012); and the here-described leonardsenite.

Leonardsenite was also first reported as a potentially new mineral by Jakobsson et al. (2008), who referred to it as "mineral HR". In the list of unnamed minerals maintained by the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC) (Smith & Nickel 2007), it is listed under valid minerals with the code UM2008-28-F:AlHMgO. The new mineral and its name have been approved by the CNMNC (IMA2011-059, Mitolo *et al.* 2011).

The mineral is named leonardsenite in honor of Dr Erik Leonardsen (1934–), the former leader of the X-Ray Diffraction Laboratory of the Geological Institute, University of Copenhagen, in acknowledgement of his major contribution to definition of a number of new minerals and especially his voluminous work on the diffraction characterization of the fumarolic minerals from Icelandic volcanoes.

The holotype is deposited in the mineral collection of the Icelandic Institute of Natural History, Gardabaer, Iceland, under sample number NI 12256 (Eldfell). Other samples, in which leonardsenite has been identified (cotype specimens), have the numbers NI 20630 (Eldfell) and NI 15509, NI 17067, NI 17073, and NI 17074 (Hekla). Part of the holotype is also deposited at the Museum "C.L. Garavelli", Dipartimento di Scienze della Terra e Geoambientali, Università di Bari, Italy, catalogue number 14/nm-V28.

OCCURRENCE AND PHYSICAL PROPERTIES

The holotype specimen of leonardsenite was collected on April 30, 1988, as a fumarolic encrustation from the northeast rim of the main crater of Eldfell volcano, Heimaey Island, Iceland (Fig. 1). Associated phases are jakobssonite (Balić-Žunić *et al.* 2012)

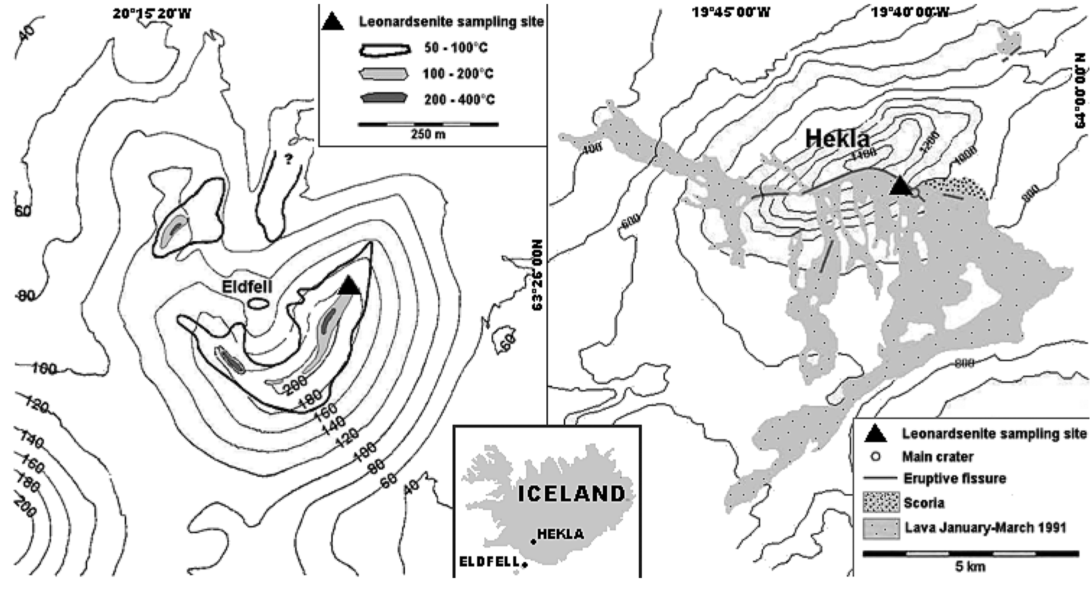

FIG. 1. Leonardsenite sampling sites at Eldfell and Hekla volcanoes, Iceland (modified after Jakobsson *et al.* 2008).

and, subordinately, anhydrite, ralstonite, jarosite and anhydrous AlF_3, and oskarssonite (IMA 2012-088, Jacobsen *et al.* 2013). The mineral was also identified in an additional sample collected from the same locality on November 15, 1995, in association with opal-A, ralstonite, jakobssonite, and other still unidentified minerals. The subsurface temperature measured at the time of this last sampling was less than 100 ºC.

Successively, leonardsenite was found in one sample of fumarolic encrustation collected on September 16, 1992, and in three samples collected on September 15, 1993, from a fumarole field along the fissure above the eastern main crater of the 1991 Hekla eruption (Fig. 1). This locality was, however, completely covered by new scoria produced by the 2000 Hekla eruption, which hid the entire fumarole field. In samples from Hekla, leonardsenite is associated with ralstonite, opal-A, jakobssonite, malladrite, fluorite, and other still unidentified minerals. The ground temperature where leonardsenite was collected ranged from 170 to 190 °C.

Leonardsenite forms soft and fragile white crusts composed of granular and columnar crystals up to 20 μm in length (Fig. 2). Comparing the SEM observations with the calculated shape of the crystal according to the Donnay-Harker law (Donnay & Harker 1937), we can conclude from a perfect match to the theoretically predicted shape that the most common forms are {011} and {101} (Fig.3). The *a:b:c* ratio calculated from the unit-cell parameters is 0.697:1:0.673.

The streak is white and the luster is earthy, probably due to the fine-grained aggregates of minute crystals.

Fluorescence, hardness, and other optical properties could not be measured due to the small size of the crystals and the admixture with other phases. The intimate mixture with other mineral species also prevented the experimental determination of density. The density calculated from the empirical formula and the single-crystal cell data is 2.31 g/cm^3.

The mean refractive index was calculated using the method proposed by Korotkov & Atuchin (2008). Taking into account the empirical chemical formula, the mean refractive index of leonardsenite should be $n = 1.38$. According to the authors of the method, averaged possible error of the calculation is about 12% for non-oxides.

CHEMICAL COMPOSITION

The electron microscope used for this research was a S360 Cambridge Scanning Electron Microscope coupled with an Oxford-Link Ge ISIS Energy Dispersive Spectrometer equipped with a Super Atmosphere Thin Window ©, since this allows better detection of light elements. An energy dispersive spectrometer (EDS) was chosen for quantitative analyses of the small-sized crystals, instead of a wavelength-dispersive spectrometer (WDS), because it allows analyses at a non-critical working distance (Ruste 1979, Acquafredda & Paglionico 2004, Balić-Žunić *et al.* 2012) with a lower probe current. The non-critical working distance permits ED quantitative analyses directly from crystal surfaces that are not totally flat, that is when they lack the necessary focusing WD geometry. Moreover, the micrometer sized crystals of leonardsenite quickly decompose at a probe current exceeding 3 nA, which generates few X-rays easily detectable only by an ED detector.

The investigated sample of leonardsenite was sputtered with a 30 nm-thick carbon film to perform SEM-EDS observations and microanalysis. Operating conditions of the SEM were: 15 kV accelerating potential, 500 pA probe current, 2500 cps as average count rate on the whole spectrum, typical counting time 100s. X-ray intensities were converted to wt.% by the ZAF-4/FLS quantitative analysis software support of Oxford-Link Analytical (UK), which allows matching of the peaks of the standards with those of the analyzed

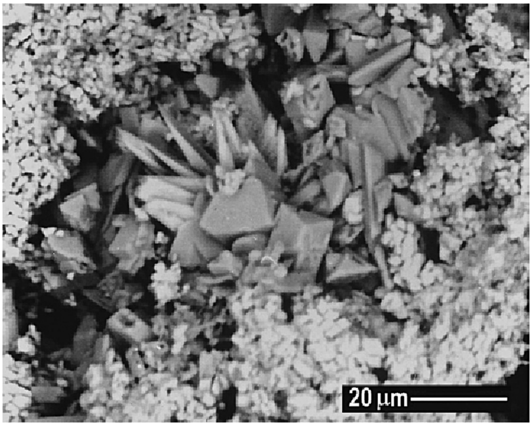

FIG. 2. SEM-BSE image of leonardsenite from Eldfell volcano. The larger columnar crystals and fine granular aggregates are associated with acicular crystals of jakobssonite (sample NI12256, holotype).

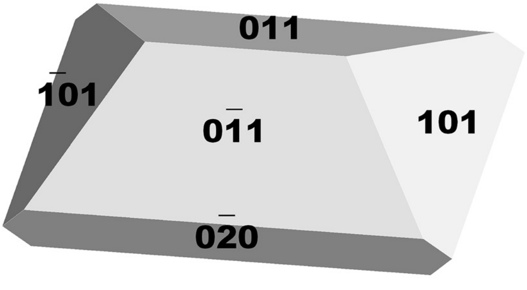

FIG. 3. Idealized drawings of a typical crystal of leonardsenite.

mineral, taking into account both the relative contribution of the matrix and the occasional partial or complete overlap among peaks of different elements.

The investigated sample consists of granular and columnar crystals of leonardsenite, up to 20 μm in length, often associated with acicular and microgranular crystals of jakobssonite (Fig. 2). The analytical results (mean of 6 analyses) are reported in Table 1. The empirical formula, calculated on the basis of two cations (Mg + Al) *pfu*, is: $Mg_{1.00}Al_{1.00}[F_{4.64}(OH)_{0.36}]_{\Sigma 5.00}(H_2O)_{1.29}$. The simplified formula is $MgAlF_5(H_2O)_2$, which ideally requires Mg 13.33, Al 14.80, H 2.22, O 17.55, and F 52.11 wt.%.

DIFFRACTION PROPERTIES AND CRYSTAL STRUCTURE DESCRIPTION

X-ray powder diffraction

X-ray powder diffraction data (XRPD) were collected using a Bruker-AXS D8 diffractometer with Bragg-Brentano geometry and a primary-beam Ge(111) monochromator, using Cu$K\alpha_1$ radiation (λ = 1.5406 Å) and a fixed divergence slit. Although leonardsenite appears in a number of samples from the two localities (Fig. 1), it was not possible, even with very small amounts of powder, to separate a pure leonardsenite phase for the powder diffraction analysis. The only sample in which leonardsenite seems to be the main component was obtained from a somewhat harder and more compact core of a completely white, rounded fragment, approximately 8 mm in diameter, from sample NI 12256 (holotype). The powdery outer part of this piece showed generally the same mineralogical composition, but with a larger amount of other phases. The best powder diagram of leonardsenite also contains jakobssonite and the mineral "HB" (Fig. 4). Given these circumstances, we based our powder diffraction analysis on a combination of the Bruker-AXS programs EVA for the experimental determination of the positions and intensities of the diffraction maxima and TOPAS for the determination of indices of reflections and the crystal lattice parameters through the Rietveld method. For the latter we used the crystal structure data of Weil & Werner (2001) and Hemon & Courbion (1991) for leonardsenite and jakobssonite, respectively. Due to the significant amount of unknown components in the

TABLE 1. CHEMICAL COMPOSITION OF LEONARDSENITE

Constituent	wt.%	Range	SD	Probe standard
Mg	14.66	13.74 – 15.14	0.49	periclase
Al	16.16	15.10 – 16.84	0.66	corundum
F	52.98	51.37 – 54.21	1.02	synth. LiF
O	15.88	15.13 – 16.40	0.43	periclase
H*	1.78			
Total	101.46			

*Calculated from the OH required for charge neutrality plus remaining O as H_2O.

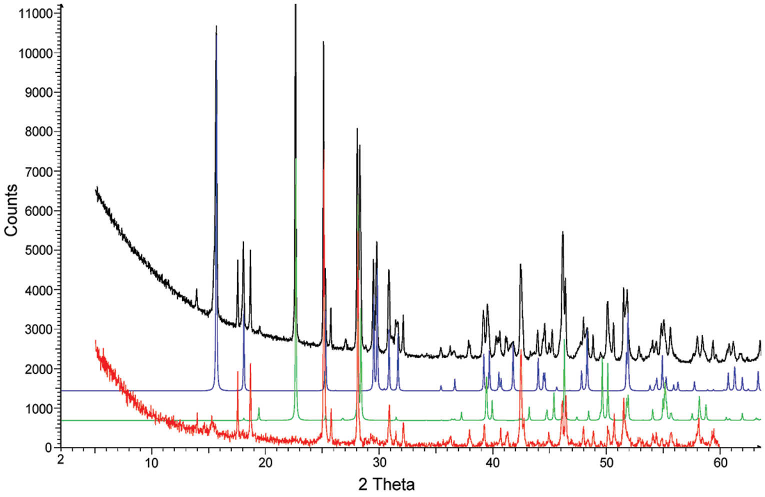

FIG. 4. X-ray powder diffraction diagram of leonardsenite with jakobssonite and mineral "HB" (Jakobsson et al. 2008; UM2008-//-?[6]) (in black). The theoretical diagrams of leonardsenite and jakobssonite obtained in Rietveld refinement are represented in blue and green, respectively. The experimental diagram of almost pure mineral "HB" is represented in red, for comparison.

diagram and consequent large residuals, no refinement of atomic parameters was completed. A comparison of the experimental diagram with the data from the Powder Diffraction Files PDF 39-0665 (Feki *et al.* 1986) and PDF 71-3013 (Weil & Werner 2001) referring to $MgAlF_5(H_2O)_{1.5}$ and $MgAlF_5(H_2O)_2$, respectively, is shown in Table 2. The experimental X-ray powder diffraction pattern of the leonardsenite holotype and the theoretical diagram based on the Rietveld fitting are shown in Figure 4.

Crystal structure

Through a good match of our powder diffraction data with those of Feki *et al.* (1986) and those based on the crystal structure refinement (Weil & Werner 2001), we conclude that basically the same phase was observed in all cases. There remains an interesting question about the amount of water present in the structure.

Leonardsenite contains isolated chains of $[AlF_6]$ octahedra which run parallel to the *a* axis (Figs. 5, 6). As previously reported by Weil & Werner (2001) for the analogous synthetic phase, in the leonardsenite structure the chains of $[AlF_6]$ are kinked parallel to the (010) plane and are in pairs bridged by individual $[MgF_4(H_2O)_2]$ octahedra. The Mg coordination octahedra bridge pairs of adjacent Al octahedra in a chain (Fig. 5) and have water molecules in *trans* positions (Fig. 6). The thermal analysis of Weil & Werner (2001) confirms the amount of water determined in their crystal structure analysis (two molecules *pfu*). $MgAlF_5(H_2O)_2$ totally dehydrates at temperatures above 300 °C to give anhydrous $MgAlF_5$ with a different structure type than the hydrous phase. The DSC curve shows a strong and sharp endothermal peak at 300 °C, but also a broad and weaker peak at about 250 °C, corresponding to the loss of about one molecule of water.

Although the features of the TG/DSC diagram (Weil & Werner 2001), the chemical data of Feki *et al.* (1986), and the present study might indicate the possibility of a partial dehydration of leonardsenite, it cannot be definitely confirmed on the basis of the crystal structure. The two water molecules complete the coordination sphere of Mg to the usual octahedron and the bond valence calculation using the formula of Brown & Altermatt (1985) and the updated parameters of Brese & O'Keeffe (1991) reveal that their bond strengths are comparable to the fluorine atoms

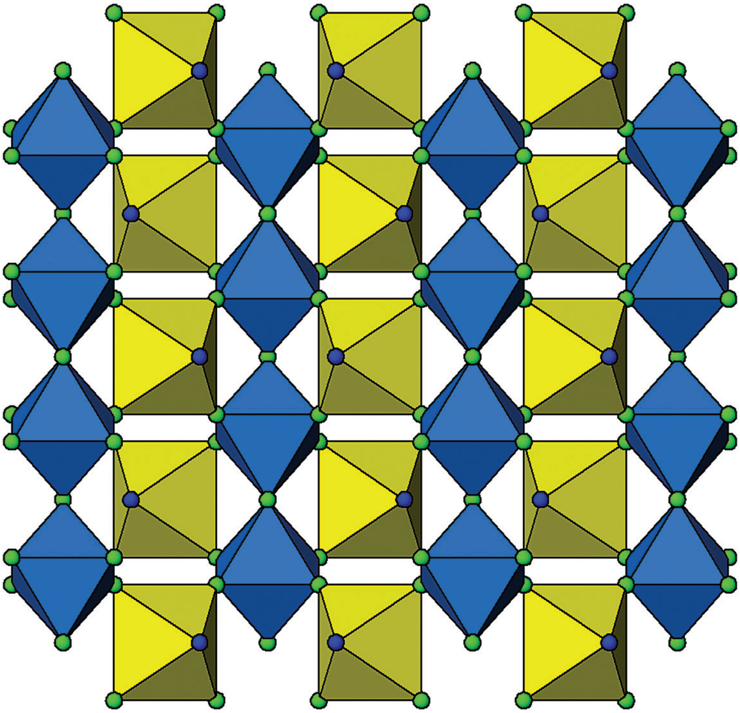

FIG. 5. Projection of the leonardsenite structure along the *c* axis (*b* axis horizontal). $[AlF_6]$ octahedra are blue and $[MgF_4(H_2O)_2]$ are yellow. Fluorine atoms are represented as green spheres and H_2O molecules as blue spheres.

TABLE 2. X-RAY POWDER DIFFRACTION DATA OF LEONARDSENITE (HOLOTYPE SAMPLE) COMPARED WITH THE SYNTHETIC $MgAlF_5{\cdot}1.5H_2O$ (PDF 39-0665[1]) AND $MgAlF_5{\cdot}2H_2O$ (PDF 71-3013[2])

leonardsenite				Synthetic PDF 39-0665[1]		Synthetic PDF 71-3013[2]	
I/I$_o$	*d*$_{meas.}$	*d*$_{calc.}$	*hkl*	*I/I$_o$*	*d*$_{meas.}$	*I/I$_o$*	*d*$_{calc.}$
7	*6.37*		*HB*				
100	**5.66**	**5.65**	**011**	**100**	**5.64**	**100**	**5.63**
23	*5.06*		*HB*			0.3	5.07
29	**4.92**	**4.90**	**101**	**28**	**4.89**	**21**	**4.89**
27	*4.76*		*HB*				
3	*4.56*		*J*				
143	*3.93*		*J*				
103	*3.55*		*HB*				
27	**3.53**	**3.53**	**200**	**26**	**3.52**	**20**	**3.52**
13	*3.46*		*HB*			0.1	3.39
3	*3.29*		*S?*				
76	*3.18*		*HB+J*				
70	*3.15*		*J*				
2	*3.10*		*?*				
31	**3.03**	**3.02**	**031**	**36**	**3.03**	**22**	**3.02**
38	**3.00**	**2.99**	**211**	**53**	**3.00**	**30**	**2.99**
			112			1	2.92
29	2.90	2.89	220+*HB*	21	2.90	15	2.90
12	*2.84*		*HB*				
12	2.83	2.83	022	16	2.83	13	2.82
14	*2.79*		*HB*				
3	2.53	2.53	040	2	2.53	1	2.53
4	*2.477*		*HB*				
2	2.456	2.450	202	6	2.452	3	2.45
6	*2.374*		*HB*				
5	*2.366*		*HB*				
16	**2.297**	**2.295**	**231**	16	2.301	9	2.30
18	2.277	2.269	132+*J*	13	2.279	9	2.27
				13	2.271		
8	*2.237*		*?*				
8	2.227	2.223	301	9	2.228	5	2.22
9	2.219	2.216	013+*HB*			3	2.20
8	*2.193*		*HB*				
7	*2.187*		*HB*				
6	2.162	2.162	103	9	2.161	10	2.15
32	*2.129*		*HB*				
31	*2.125*		*HB*				
14	*2.119*		*HB*				
2	*2.086*		*J*				
10	2.059	2.055	240	10	2.060	8	2.06
7	2.039	2.035	321	9	2.038	4	2.04
12	2.031	2.031	042+*J*			4	2.03
5	*2.015*		*HB*				
10	*2.003*		*J*				
43	*1.965*		*J+HB*			1.	1.98
28	*1.955*		*HB*			0.2	1.94
6	1.903	1.901	312	16	1.894	5	1.90
15	*1.894*		*HB*				
11	1.883	1.884	033			13	1.88
		1.876	213			7	1.87
8	*1.864*		*HB*				
2	*1.839*		*J*				
20	*1.819*		*J+HB*				
13	*1.802*		*HB*				

25	*1.773*		*HB*				
19	**1.766**	**1.764**	**400**+*J*	**32**	**1.765**	9	1.77
24	**1.762**	**1.760**	**242**+*J*			19	1.76
5	*1.730*		*HB*				
7	1.695	1.703	004+*HB*			1	1.69
		1.700	251			0.2	1.70
6	1.686	1.689	152+*HB*	4	1.689	2	1.69
		1.686	060				
		1.684	411	6	1.682	4	1.69
13	1.673	1.670	341			8	1.67
15	1.666	1.665	420+*J*	11	1.664	5	1.67
		1.662	233+*J*			3	1.66
12	*1.650*	*1.643*	*HB*+*J*+143			2	1.64
			303			2	1.63
			114			1	1.63
3	1.597	1.594	161	2	1.598	2	1.60
9	*1.588*		*HB*+*J*				
9	*1.577*		*J*				
7	*1.555*		*HB*			0.4	1.55
2	*1.547*		*HB*				
6	1.522	1.523	431			4	1.53
		1.521	260				
7	1.513	1.511	062			4	1.51
		1.511	053				
3	1.500	1.496	422			3	1.50
8	1.463	1.468	224			4	1.46

[1]Feki *et al.*, 1986; [2]Weil and Werner, 2001; [3]Balić-Žunić *et al.*, 2012.
The eight strongest reflections of leonardsenite are given in bold. The reflections of jakobssonite[3] [*J*], mineral "HB" (Jakobsson et al. 2008; UM2008-//-?[6]) [*HB*], and tentative sellaite [*S*] are given in italics.

bonded to Mg. A partial loss of water departing from the full coordination of the Mg atom should therefore be expected to introduce significant changes in atomic positions, but the diagram reported by Feki *et al.* (1986) and our results do not show any significant differences from the diagram reported by Weil & Werner (2001), which was calculated from the crystal structure data of $MgAlF_5(H_2O)_2$.

DISCUSSION

Leonardsenite, with ideal formula $MgAlF_5(H_2O)_2$, is a complex alkaline earth aluminum fluoride which was found as a volcanic encrustation at Eldfell and Hekla volcanoes. Both these volcanoes are characterized by high fluorine content in the volcanic gasses discharging from fumaroles (Oskarsson 1981), as confirmed by the presence of fluorides and fluorosilicates among sublimates and fumarole encrustations.

Investigation by Langmyhr & Kringstad (1966) indicated that the decomposition of a variety of ordinary silicate rocks in concentrated solutions of hydrofluoric acid results in the formation of fluoride compounds among which ralstonite, $Na_xMg_xAl_{2-x}(F,OH)_6{\cdot}H_2O$, and leonardsenite, $MgAlF_5(H_2O)_2$, are abundant. According to this genetic mechanism, at Eldfell and Hekla volcanoes, the volcanic fluorine-rich vapors may decompose the lava minerals previously formed (Jakobsson *et al.* 2008), and the formation of new phases may occur.

The new mineral is isostructural with a number of $M^{II}FeF_5(H_2O)_2$ compounds, with M = Zn, Mn, Fe, Co, Ni, and with several $M^{II}M^{III}F_5(H_2O)_2$ compounds (Table 3). These phases are known as inverse weberites because of the opposite roles that M^{II} and M^{III} play in the crystal structure compared to Na_2MgAlF_7 weberite (Byström 1944, Knop *et al.* 1982). Further differences from weberite are: the absence of alkaline (Na) atoms and corresponding vacancies in the structure, and the substitution of two F by water molecules.

Obviously, additional investigation is desirable to better define the possible water content and the variable stoichiometry of leonardsenite. Until then, and considering the low accuracy of the chemical analysis that could be applied on the available natural samples, we assume that the best idealized formula for the mineral is $MgAlF_5(H_2O)_2$.

Among the other Mg fluoride minerals, sellaite, MgF_2, is known both from hydrothermal/pneumatolitic deposits and from fumarolized areas. It has a rutile-type structure. Besides weberite, Mg builds complex fluorides such as: neighborite, $NaMgF_3$, and usovite, $Ba_2CaMgAl_2F_{14}$, both known as hydrothermal minerals; unnamed $KMgF_3$, reported from volcanic exhalative deposits (UM1960-02-F:KMg, Smith & Nickel 2007);

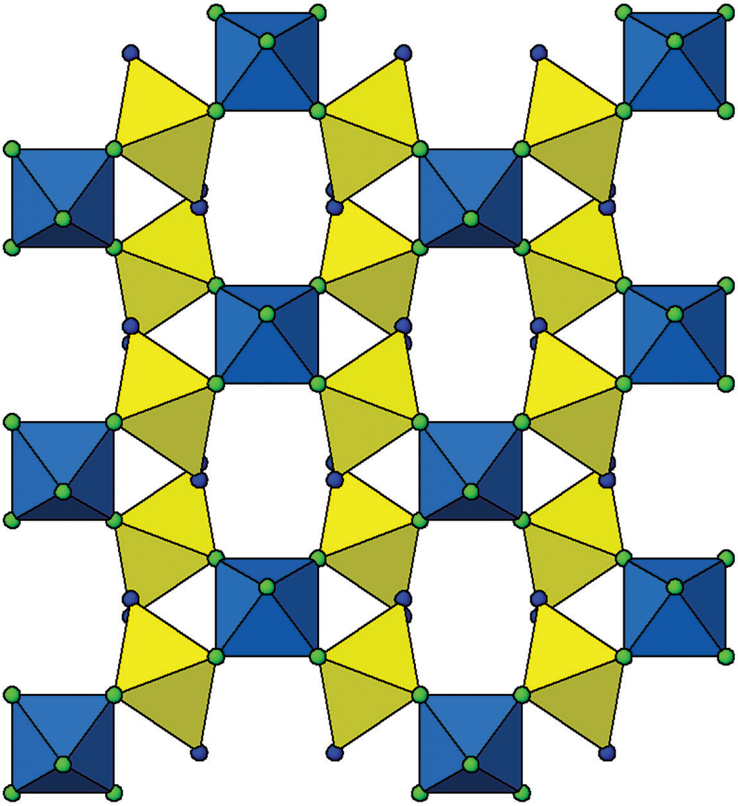

FIG. 6. Projection of the leonardsenite structure along the *a* axis (*b* axis horizontal).

and $MgAlF_5$ (Weil & Werner 2001) and $MgAl_2F_8(H_2O)_2$ (Weil *et al*. 2002), which have not been reported from nature, to the best of our knowledge.

Finally, leonardsenite belongs to the group of fluorides with interesting catalytic and optical properties, with applications ranging from phosphors to lasers (Rubio 1991, Joubert *et al*. 2001, Weil & Werner 2001, Weil *et al*. 2002).

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TABLE 3. COMPARISON OF LEONARDSENITE AND WEBERITE-GROUP COMPOUNDS

Compound	*a* (Å)	*b* (Å)	*c* (Å)	Space group	References
leonardsenite	7.055(1)	10.117(2)	6.813(1)	*Imma*	this work
$MgAlF_5(H_2O)_2$	7.0637(7)	10.131(1)	6.7745(7)	*Imma*	Weil & Werner 2001
$MgAlF_5(H_2O)_2$	7.057(2)	10.125(4)	6.798(2)	*Imma*	Subramanian *et al.* 2006
$ZnAlF_5(H_2O)_2$	7.141(2)	10.308(4)	6.645(2)	*Imma*	ibid.
$CoAlF_5(H_2O)_2$	7.193(2)	10.352(4)	6.608(2)	*Imma*	ibid.
$MnAlF_5(H_2O)_2$	7.229(2)	10.487(4)	6.816(2)	*Imma*	ibid.
$CdAlF_5(H_2O)_2$	7.331(2)	10.639(4)	6.829(2)	*Imma*	ibid.
$ZnGaF_5(H_2O)_2$	7.380(2)	10.600(4)	6.584(2)	*Imma*	ibid.
$MnGaF_5(H_2O)_2$	7.471(2)	10.735(4)	6.720(2)	*Imma*	ibid.
$CdGaF_5(H_2O)_2$	7.603(2)	10.875(4)	6.718(2)	*Imma*	ibid.
$ZnVF_5(H_2O)_2$	7.486(2)	10.756(4)	6.589(2)	*Imma*	ibid.
$MnVF_5(H_2O)_2$	7.607(2)	10.912(4)	6.728(2)	*Imma*	ibid.
$Fe_2F_5(H_2O)_2$	7.489(7)	10.897(8)	6.671(6)	*Imma*	Hall *et al.* 1977
$ZnFeF_5(H_2O)_2$	7.475(1)	10.766(1)	6.594(1)	*Imma*	Laligant *et al.* 1986
$MnFeF_5(H_2O)_2$	7.5635(2)	10.901(1)	6.7319(2)	*Imma*	Laligant *et al.* 1987
weberite Na_2MgAlF_7	7.051(1)	9.968(2)	7.285(1)	*Imm*2	Knop *et al.* 1982
Na_2NiFeF_7	7.245(1)	10.320(1)	7.458(1)	*Imm*2	Haegele *et al.* 1978
Na_2MgInF_7	7.345(1)	10.345(1)	7.553(1)	*Pmnb**	Caramanian *et al.* 2001
Na_2NiGaF_7	7.161(1)	10.216(2)	7.409(1)	*Imma*	Dahlke *et al.* 1998

*In the original work the orientation of the crystallographic axes was chosen according to *Pnma.*

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