

JØRGENSENITE, $\text{Na}_2(\text{Sr},\text{Ba})_{14}\text{Na}_2\text{Al}_{12}\text{F}_{64}(\text{OH},\text{F})_4$, A NEW ALUMINOFUORIDE MINERAL FROM IVIGTUT, GREENLAND

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ABSTRACT

Jørgensenite, $\text{Na}_2(\text{Sr},\text{Ba})_{14}\text{Na}_2\text{Al}_{12}\text{F}_{64}(\text{OH},\text{F})_4$, is a new aluminofluoride mineral from the Ivigtut cryolite deposit at Ivigtut, Greenland. It occurs in fissure fillings within the main cryolite mass, and in crystal-lined cavities containing fan-shaped aggregates (up to 2 mm across) of jørgensenite overgrown by jarlite. It also occurs as grains up to 10 mm across with stemonite. It is veined by stemonite, but also veins and cements irregular fragments of stemonite. Jørgensenite is transparent, colorless to white, with a colorless to white streak, a vitreous luster and an uneven fracture; it shows no fluorescence. It is brittle, H 3½–4, D_{meas} 3.89(1) g/cm³, D_{calc} 3.94 g/cm³. In plane-polarized light, it is colorless, nonpleochroic, biaxial negative, α 1.436(1), β 1.442(1), γ 1.442(1), $2V$ 0–5°, $\beta = b$, and without visible dispersion. Crystals are elongate along the b axis; no twinning was observed. Jørgensenite is monoclinic, space group $C2/m$, with the following unit-cell dimensions, refined from powder X-ray-diffraction data: a 16.046(1), b 10.971(1), c 7.281(1) Å, β 101.734(6)°, V 1254.9(3) Å³, $Z = 1$. The axial ratios, calculated from the refined cell-parameters, are $a:b:c = 1.4634:1:0.6631$. The ten strongest reflections in the X-ray powder-diffraction pattern [d in Å (l,h,k)] are: 7.844(8,200), 3.643(9,311), 3.453(10,112), 3.193(10,420), 3.112(9,421), 2.998(5,330), 2.989(9,022), 2.220(8,441), 2.173(9,150), and 2.001(8,801). Chemical analysis by electron-microprobe and analytical SEM gave Na 3.25, K 0.30, Mg 0.38, Ca 0.28, Sr 32.76, Ba 8.63, Al 10.97, F 42.50, H₂O_{calc} 1.22, sum 100.29 wt%; the presence of OH in the structure was confirmed by microbeam infrared spectroscopy. The formula unit, calculated on the basis of 12 Al atoms per formula unit, is $\text{Na}_2(\text{Sr}_{11.03}\text{Ca}_{0.21}\text{Ba}_{1.85}\text{K}_{0.23}\text{Na}_{0.63})(\text{Na}_{1.54}\text{Mg}_{0.46})\text{Al}_{12}\text{F}_{64}[(\text{OH})_{2.00}\text{F}_{2.00}]$. Jørgensenite is isostructural with jarlite, ideally $\text{Na}_2(\text{Sr},\text{Na},\text{F})_{14}(\text{Mg},\text{Ca})_2\text{Al}_{12}\text{F}_{64}(\text{OH},\text{H}_2\text{O})_4$, and is named after Vilhelm Jørgensen (1844–1925), cofounder (with G.A. Hagemann) of the cryolite factory at Ivigtut in 1870.

Keywords: jørgensenite, new mineral, chemical analysis, X-ray powder-diffraction pattern, optical properties, jarlite, Ivigtut, Greenland.

SOMMAIRE

La jørgensenite, $\text{Na}_2(\text{Sr},\text{Ba})_{14}\text{Na}_2\text{Al}_{12}\text{F}_{64}(\text{OH},\text{F})_4$, nouvelle espèce minérale, est un aluminofluorure provenant du gisement de cryolite d'Ivigtut, au Groënland. On trouve ce minéral en remplissage de fissures dans la masse principale de cryolite, et dans des cavités tapissées de cristaux, parmi lesquels des agrégats fibroradiés jusqu'à 2 mm en largeur de jørgensenite recouverte de jarlite. On la trouve aussi en cristaux atteignant 10 mm de taille associée à la stemonite. Elle est recoupée par la stemonite, mais elle recoupe et cimente elle-même des fragments de stemonite. La jørgensenite est transparente, incolore à blanche, avec une rayure semblable, un éclat vitreux et une fracture inégale. Elle n'est pas fluorescente. Elle est cassante, d'une dureté entre 3½ et 4, avec une densité mesurée de 3.89(1) et une densité calculée de 3.94. En lumière simplement polarisée, elle est incolore, non pléochroïque, biaxe négative, α 1.436(1), β 1.442(1), γ 1.442(1), $2V$ 0–5°, $\beta = b$, sans dispersion visible. Les cristaux sont allongés selon l'axe b ; nous n'avons pas observé de macles. La jørgensenite est monoclinique, groupe spatial $C2/m$, et possède les paramètres réticulaires suivants, tels qu'affinés à partir des données de diffraction X obtenues sur poudre: a 16.046(1), b 10.971(1), c 7.281(1) Å, β 101.734(6)°, V 1254.9(3) Å³, $Z = 1$. Les rapports des axes, calculés à partir de ces paramètres, sont: $a:b:c = 1.4634:1:0.6631$. Les dix raies les plus intenses du cliché de diffraction, méthode des poudres, [d en Å (l,h,k)] sont:

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7.844(8,200), 3.643(9,311), 3.453(10,11 $\bar{2}$), 3.193(10,420), 3.112(9,42 $\bar{1}$), 2.998(5,330), 2.989(9,022), 2.220(8,44 $\bar{1}$), 2.173(9,150), et 2.001(8,80 $\bar{1}$). Une analyse chimique obtenue à la microsonde électronique et par dispersion d'énergie avec microscope électronique à balayage a donné Na 3.25, K 0.30, Mg 0.38, Ca 0.28, Sr 32.76, Ba 8.63, Al 10.97, F 42.50, H₂O_{calc} 1.22, total 100.29% en poids; la présence d'hydroxyle dans la structure a été confirmée par micro-spectroscopie dans l'infrarouge. L'unité formulaire, calculée sur une base de douze atomes de Al, est Na₂(Sr_{11.03}Ca_{0.21}Ba_{1.85}K_{0.23}Na_{0.63})(Na_{1.54}Mg_{0.46})Al₁₂F₆₄[(OH)_{2.00}F_{2.00}]. La jørgensenite possède la structure de la jarlite, c'est-à-dire de façon idéale Na₂(Sr,Na,□)₁₄(Mg,□)₂Al₁₂F₆₄(OH,H₂O)₄. Le nom honore Vilhelm Jørgensen (1844–1925), co-fondateur (avec G.A. Hagemann) de l'usine de cryolite à Ivigtut en 1870. (Traduit par la Rédaction)

Mots-clés: jørgensenite, nouvelle espèce minérale, analyse chimique, données de diffraction X, méthode des poudres, propriétés optiques, jarlite, Ivigtut, Grønland.

INTRODUCTION

Jarlite is an aluminofluoride mineral first described by Bøggvad (1933) from the cryolite quarry at the Ivigtut cryolite deposit, Greenland. It occurs as flat fan-shaped aggregates of crystals in association with thomsenolite and minor gearksutite. Bøggvad (1933) also reported a mineral similar to jarlite, "metajarlite", intergrown with chiolite and associated with minor cryolite, fluorite, topaz and pyrite. Brosset (1942) and Ferguson (1947) concluded that jarlite and "metajarlite" are isostructural, and that the previously assigned formula of jarlite, NaSr₂Al₃F₁₆, is wrong. Hawthorne (1983) solved the crystal structure of jarlite and assigned it the formula Na₂(Sr,Na,□)₁₄(Mg,□)₂Al₁₂F₆₄(OH,H₂O)₄. Pauly & Nielsen (1992) did detailed electron-microprobe work on jarlite and "metajarlite". They found jarlite crystals and grains to be composite, with a core surrounded by a mantle, and showed that the two are significantly different in composition; the mantle has essential Mg, in agreement with the formula of jarlite, whereas the

core does not. The composition of the dendritically developed jarlite (called "metajarlite") also agrees with the jarlite formula. The Mg-free core is thus a new mineral; we name this species jørgensenite after Vilhelm Jørgensen (1844–1925), founder of the cryolite factory (together with G.A. Hagemann) in 1870, and father of C.F. Jarl. The new mineral and the mineral name have been approved by the International Mineralogical Association Commission on New Minerals and Mineral Names. Type material is deposited at The Geological Museum, University of Copenhagen, Copenhagen, Denmark, catalogue number 1996.168.

PHYSICAL AND OPTICAL PROPERTIES

Jørgensenite is white and translucent, with a colorless to white streak and a vitreous luster. Crystals are elongate along the *b* axis; no twinning was observed. Jørgensenite is overgrown by jarlite in optical continuity, with a sharp optical boundary between the two phases. They form curved grains (Fig. 1) or fan-shaped



FIG. 1. Elongate grains of jørgensenite, greyish with a black rim, overgrown by jarlite; crossed polars, magnification 70X.



FIG. 2. A fan-shaped aggregate of jørgensenite crystals overgrown by jarlite; crossed polars, magnification 60X.

groups of crystals (Fig. 2). Jørgensenite shows no fluorescence under long- or short-wave ultraviolet light. It has a Mohs hardness of 3½–4, no cleavage or parting, and is brittle with an uneven fracture. The density, measured by suspension in Clerici solution, is 3.89(1) g/cm³, compared with a calculated density of 3.94 g/cm³.

Jørgensenite is colorless in transmitted light. It is biaxial negative, with indices of refraction α 1.436(1), β 1.442(1), γ 1.442(1), measured in white light; $Y = \beta$, $2V_z = 0-5(5)^\circ$, $2V_{\text{calc}} = 0^\circ$. Dispersion was not observed, and there is no pleochroism.

CHEMICAL COMPOSITION

Jørgensenite was analyzed with an electron microprobe operating in wavelength-dispersion mode. The following standards were used: weberite (Na, Mg, Al), orthoclase (K), wollastonite (Ca), bøggildite (Sr) and barite (Ba). The concentration of F was measured by standardless analysis on an analytical SEM operating in the wavelength-dispersion mode. The amount of H₂O was not determined, but the presence of OH was confirmed by microbeam infrared spectroscopy. The chemical composition and unit formula calculated on the basis of 12 Al *apfu* (atoms per formula unit) are given in Table 1. The unit formula was calculated in this way as the amount of F in the formula is variable owing to OH-for-F substitution. The empirical formula (Table 1) may be generalized to Na₂(Sr,Ba)₁₄(Na,Mg)₂Al₁₂F₆₄(OH,F)₄. The end-member formula may be written as Na₂Sr₁₄Na₂Al₁₂F₆₄(OH,F)₄; it is not possible to choose an ideal composition for the (OH,F)₄ part of the end-member formula as OH is equal to F in the empirical formula (Table 1).

TABLE 1. CHEMICAL COMPOSITION* AND FORMULA UNIT (*apfu*) OF JØRGENSENITE

wt%		UNIT FORMULA**	
Al	10.97	Al	12
Mg	0.38		
Ca	0.28	Mg	0.46
Sr	32.76	Na	1.54
Ba	8.63	Σ	2.00
Na	3.25		
K	0.30	Sr	11.03
F	42.50	Ca	0.21
(H ₂ O)*	1.22	Ba	1.85
	<u>100.29</u>	K	0.23
		Na	0.63
		Σ	13.95
		Na	2.00
		F	66.00
		OH	2.00

* mean of 11 determinations;

** calculated on the basis of 12 Al *apfu*;

* calculated for OH + F = 68 *apfu*.

TABLE 2. INDEXED POWDER-DIFFRACTION PATTERN AND REFINED CELL-DIMENSIONS FOR JØRGENSENITE

<i>l</i>	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>hkl</i>	<i>l</i>	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>hkl</i>
8	7.844	7.855	2 0 0	3	2.157	2.156	2 0 3
1	7.124	7.129	0 0 1	2	2.140	2.140	5 3 2
3	5.831	5.833	1 1 1	2	2.076	2.076	4 4 1
3	5.806	5.811	2 0 1	1	2.062	2.062	1 5 1
2	4.724	4.726	3 1 0	1	2.031	2.031	2 4 2
1	4.502	4.497	2 2 0	1	2.024	2.024	3 5 0
3	4.345	4.347	0 2 1	8	2.001	2.000	8 0 1
1	4.019	4.021	2 2 1	1	1.992	1.992	7 1 1
1	3.925	3.928	4 0 0	1	1.971	1.970	6 0 3
1	3.780	3.780	4 0 1	3	1.964	1.964	8 0 0
9	3.643	3.643	3 1 1	1	1.936	1.936	1 3 3
4	3.560	3.562	1 3 0	1	1.913	1.913	7 3 0
1	3.528	3.527	2 0 2	1	1.901	1.901	6 4 1
10	3.453	3.454	1 1 2	3	1.879	1.879	1 5 2
2	3.246	3.247	1 3 1	1	1.871	1.871	4 0 3
10	3.193	3.194	4 2 0	1	1.853	1.853	5 3 2
2	3.178	3.178	4 0 1	1	1.830	1.830	5 3 3
4	3.136	3.136	3 1 2	1	1.803	1.803	7 1 3
4	3.129	3.129	3 1 3	1	1.795	1.795	5 5 1
9	3.112	3.113	4 2 1	2	1.787	1.787	8 2 2
3	3.022	3.021	5 1 0	1	1.737	1.737	4 4 3
5	2.998	2.998	3 3 0	1	1.724	1.724	7 1 2
9	2.889	2.889	0 2 2	4	1.711	1.712	6 2 1
3	2.867	2.867	2 2 2	1	1.698	1.698	5 5 1
3	2.956	2.956	4 0 2	1	1.666	1.666	2 0 4
2	2.986	2.986	3 3 1	1	1.646	1.646	4 6 1
3	2.744	2.743	0 4 0	1	1.624	1.624	1 3 4
2	2.654	2.655	3 3 1	1	1.616	1.616	8 4 1
1	2.637	2.638	6 0 1	1	1.602	1.601	9 3 1
1	2.602	2.602	4 2 2	1	1.584	1.584	2 2 4
1	2.564	2.565	5 1 2	1	1.580	1.580	7 5 1
1	2.376	2.376	0 0 3	1	1.567	1.566	5 3 3
3	2.365	2.366	1 1 3	1	1.551	1.551	9 1 3
2	2.247	2.245	4 0 3	1	1.530	1.530	1 7 1
8	2.220	2.220	4 4 1	3	1.516	1.516	2 4 4
1	2.210	2.210	2 2 3	1	1.502	1.502	3 7 0
9	2.173	2.173	1 5 0				

$a = 16.048(1)$, $b = 10.971(1)$, $c = 7.281(1)$ Å, $\beta = 101.734(6)^\circ$, $V = 1254.9$ Å³. Values of *d* expressed in Å.

X-RAY CRYSTALLOGRAPHY

X-ray precession photographs with Zr-filtered $\text{MoK}\alpha$ X-radiation are compatible with Laue symmetry $2/m$, and the condition for reflections to be present is $h + k = 2n$, indicating that the lattice is C -centered. Long-exposure precession photographs show no sign of any violating reflections. The possible space-groups are $C2/m$, $C2$ and Cm ; crystal-structure refinement (Hawthorne & Burns 1997) confirmed the space group $C2/m$.

A small amount of jørgensenite was ground to a grain size of approximately $2\ \mu\text{m}$. The diffraction pattern was recorded using a Guinier camera with graphite-monochromated $\text{CuK}\alpha$ X-radiation; peak intensities were estimated visually. Cell dimensions were refined, and agree closely with the results of precession photography and single-crystal structure refinement (Hawthorne & Burns 1997). The indexed powder-pattern and refined cell-dimensions are given in Table 2.

The refined structures of jarlrite and jørgensenite are graphically identical (Fig. 3). The Mg site in jarlrite, colored black in Figure 3a, is occupied by Mg and \square (vacancy), whereas the corresponding $\text{Na}(2)$ site in jørgensenite, dashed-line-shaded in Figure 3b, is occupied by Na . The type jørgensenite has significant Mg ($0.46\ \text{apfu}$) occupying the $\text{Na}(2)$ site, suggesting significant solid-solution between jarlrite and jørgensenite, although this solid-solution is complicated by significant Na -for- Sr substitution in jørgensenite. Certainly, the analytical results of Pauly & Nielsen (1992) show

significant solid-solution, but is it not clear whether this solid solution is complete.

PARAGENESIS

Jørgensenite occurs with jarlrite in two different parageneses: (1) in radiating and columnar aggregates, and (2) with stemonite. The radiating and columnar aggregates were found as fillings of meter-long, decimeter-wide fissures in the western part of the main mass of cryolite (Bøggvad 1933). They were called "columnar aggregates" because their fine-grained constituents are arranged in cm- to dm-long, mm-wide, straight lamellae delineated by cryptocrystalline topaz or fine-grained spherulitic muscovite. In addition to jørgensenite and jarlrite, strontian barite, bøggvadite, fluorite and minor pyrite are present in the aggregates. Jørgensenite overgrown by jarlrite forms slightly curved grains, a few mm long and a few tenths of a mm wide, and fan-shaped clusters within the straight lamellae of the aggregates. Although the jarlrite and the jørgensenite are in optical continuity, there is a sharp (optical) boundary between the two phases (Fig. 1).

Jørgensenite and jarlrite found within the stemonite are rather coarse grained, up to 10 mm across. Jørgensenite is distinguished from jarlrite by its small optical angle. Stemonite is veined by jørgensenite, and jørgensenite cements broken pieces of stemonite; however, veins of stemonite also cut jørgensenite. Jarlrite with a core of jørgensenite occurs as crystals lining

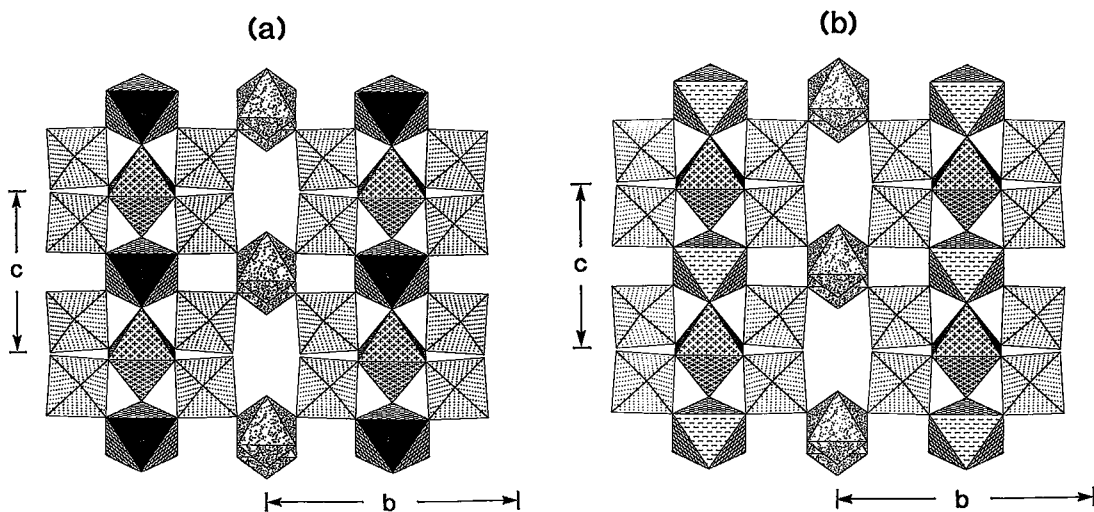


FIG. 3. Comparison of the crystal structures of (a) jarlrite and (b) jørgensenite projected onto (100); $\text{Al}(1)$ octahedra are random-dot-shaded, $\text{Al}(2)$ octahedra are regular-dot-shaded, $\text{Na}(1)$ octahedra are cross-hatched, Mg octahedra are black-faced and dashed-line shaded, and $\text{Na}(2)$ octahedra are dashed-line-shaded.

cavities in these samples, as well as in the radiating aggregates. A more detailed textural description of jarlite-jørgensenite parageneses is given by Pauly (1993).

During formation of the main siderite-cryolite and cryolite masses in the deposit, a Ca-Al-Si-F-rich residue accumulated in the deeper parts of the deposit (Pauly 1992). Subsequent explosive events, accompanied by the crystallization of cryptocrystalline topaz and the formation of the fluorite zone, led to the development of fissures and the subsequent accumulation of a Sr-Ba-rich fluid in these fissures. Prior to the introduction of the fluids, topaz precipitated on cleavage fragments of cryolite accumulated in the fissures. The columnar aggregates arose because the fluids dissolved the cryolite, and replaced it by jørgensenite together with jarlite and the accompanying minerals (Pauly 1993).

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