Matioliite, the Mg-analog of burangaite, from Gentil mine, Mendes Pimentel, Minas Gerais, Brazil, and other occurrences

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ABSTRACT

Matioliite, ideally NaMgAl₅(PO₄)₄(OH)₆·2H₂O, occurs as a secondary hydrothermal mineral in the Gentil mine granite pegmatite, Mendes Pimentel Co., Minas Gerais, Brazil. Some crystals are zoned to more Fe-rich compositions with an Fe2+:Mg ratio of approximately 1:1, corresponding to an intermediate member of the burangaite-matioliite solid-solution series. Matioliite is intimately associated with fluorapatite, crandallite, and zoned gormanite-souzalite cystals. The mineral forms prismatic to tabular crystals, up to 1 mm long. Matioliite is transparent and displays a vitreous luster; it is blue to colorless with a white streak. It is non-fluorescent. Mohs hardness is about 5. Calculated density is 2.948 g/cm³. Matioliite is biaxial negative, $\eta_{\alpha} = 1.597(2)$, $\eta_{\beta} = 1.627(2)$, $\eta_{\gamma} = 1.632(1)$ (white light), 2V (meas.) = 43(2)°, 2V (calc.) = 44°, dispersion r > v, orientation $X = \mathbf{b}$, $Z \wedge \mathbf{c} = 6°$. Pleochroism is Y > X > Z, X = light blue to colorless, Y = blue, Z = colorless. The empirical formula is $(Na_{0.94}Ca_{0.01})_{\Sigma 0.95}$ $(Mg_{0.88}Fe_{0.11}^{2+}Mn_{0.01})_{\Sigma 1.00}(Al_{4.84}Fe_{0.13}^{3+})_{\Sigma 4.97}(PO_{4})_{4.03}(OH)_{5.76}\cdot 2H_2O.$ The mineral is monoclinic, space group C2/c, a = 25.075(1) Å, b = 5.0470(3) Å, c = 13.4370(7) Å, $\beta = 110.97(3)^\circ$, V = 1587.9(4) Å³, Z = 4. Crystal-structure determination was carried out and showed it is isostructural with burangaite, dufrénite, and natrodufrénite. Both the description and the name were approved by the CNMMN-IMA (Nomenclature Proposal 2005-011). The "magnesium analog of burangaite" described from the Gold Quarry mine, Carlin-trend, Eureka County, Nevada; "burangaite" from Hochgosch, Millstätter See-Rücken, Kärnten, Austria; and "burangaite" described from Córrego Pomarolli, Linópolis, Divino das Laranjeiras, Minas Gerais, Brazil, are probably matioliite.

Keywords: Matioliite, new mineral, crystal structure, burangaite, chemical composition, Gentil mine, Mendes Pimentel, Brazil

INTRODUCTION

Matioliite, ideally NaMgAl₅(PO₄)₄(OH)₆·2H₂O, is monoclinic and isostructural with burangaite, dufrénite, and natrodufrénite. The mineral is named in honor of Paulo Anselmo Matioli (b. 1975), mineral collector, founder, and curator of the Museu de Ciências Naturais Jobas "José Bonifácio de Andrada e Silva," Santos, SP, Brazil. Matioli collected the samples used for the first official description of the new Brazilian minerals coutinhoite and matioliite. The first matioliite samples were collected in 2004 by him and Sergio Varvello. Both the description and the name were approved by the CNMMN-IMA (Nomenclature Proposal 2005-011). The type material is deposited under the number DR453 in the Museu de Geociências, Instituto de Geociências, Universidade de São Paulo, Rua do Lago, 562, 05508–080, São Paulo, SP, Brazil, and in the Museu de Ciências Naturais Jobas "José Bonifácio de Andrada e Silva," Santos, SP, Brazil.

Jensey et al. (1995) described a "burangaite-analog" at the Gold Quarry mine, Carlin-trend, Eureka County, Nevada. The mineral occurs as pale-green radiating groups and hemispheres (to 0.3 mm)

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of simple prismatic monoclinic crystals, associated with englishite, carbonate-fluorapatite, and variscite. Quantitative chemical microanalysis shows predominant Na and Mg, with about 0.5 wt% V (which, according to those authors, may be responsible for the greenish color). The lack of detectable Fe suggested to Jensey et al. (1995) that the Gold Quarry mineral might actually be "the magnesium analog of burangaite, and therefore a new species" (p. 453).

"Burangaite" from Hochgosch, Millstätter See-Rücken, Kärnten, Austria, which forms pale-blue acicular crystals having the formula Na(Mg_{0.9}Fe²⁺_{0.1})_{Σ 1.0}Al₅(PO₄)₄(OH)₆·2H₂O, was described by Walter and Ettinger (2001). Bermanec et al. (2004a, 2004b) described "burangaite" as bluish long prismatic crystals, intimately associated with brazilianite, at the Córrego Pomarolli area, Linópolis, Divino das Laranjeiras, Minas Gerais, Brazil. Chemical data, however, show that Mg predominates over Fe. The mineral of these three occurrences is probably matioliite. The remaining burangaite occurrences are the type locality (Buranga pegmatite, near Gatumba, Giseney province, Rwanda), studied by von Knorring et al. (1977) and Selway et al. (1997), and Hålsjöberg, near Ekshärad, Värmland province, Sweden (Ek and Nysten 1990).

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OCCURRENCE

Matioliite occurs as a secondary mineral in vugs from the Gentil mine granitic pegmatite, Mendes Pimentel Co., Minas Gerais, Brazil. This occurrence was studied by Scholz (2002) and Chaves et al. (in press), who identified the following phosphates: autunite, barbosalite, eosphorite, fluorapatite, frondelite, gormanite, heterosite, hureaulite, lazulite, lithiophillite, montebrasite, phosphosiderite, purpurite, scorzalite, souzalite, triphylite, triplite, and vivianite. Other minerals found in the pegmatite include: quartz, albite, microcline, muscovite, beryl, elbaite, schorl, almandine, cassiterite, columbite, tantalite, arsenopyrite, and pharmacosiderite. Roscherite-group minerals and brazilianite were also observed during this research. Matioliite is associated intimately with fluorapatite, crandallite, and zoned gormanite-souzalite cystals. Some matioliite crystals are zoned to more Fe-rich compositions with an Fe2+:Mg ratio of approximately 1:1, corresponding to an intermediate member of the burangaite-matioliite solid-solution series.

APPEARANCE AND PHYSICAL PROPERTIES

The mineral forms long, prismatic to tabular crystals, up to 1 mm (Fig. 1). Cleavage on {100} is perfect. Fracture and tenacity were not determined. Twinning was not observed. Matioliite is transparent and displays a vitreous luster; it is blue to colorless and the streak is white. It is non-fluorescent under both short (254 nm) and long wavelength (366 nm) ultraviolet radiation. The Mohs hardness is about 5. Density was not measured due to the paucity of material, but the calculated density is 2.948 g/cm³ (based on empirical formula).

OPTICAL PROPERTIES

Optical data for matioliite from Gentil mine were determined in white light. Indices of refraction were measured by immersion of grains in liquids calibrated with an Abbé refractometer. Matioliite is biaxial negative, with $\eta_{\alpha} = 1.597(2)$, $\eta_{\beta} = 1.627(2)$, $\eta_{\gamma} = 1.632(1)$ (white light), 2V (meas.) = 43(2)°, 2V (calc.) = 44°, dispersion r > v, orientation $X = \mathbf{b}$, $Z \wedge \mathbf{c} = 6°$. Pleochroism is Y > X > Z, X = light blue to colorless, Y = blue, Z = colorless.

CHEMICAL DATA

Matioliite crystals were embedded in epoxy resin and polished. The chemical analyses (17 for matioliite and 7 for the associated Fe-rich phase) were done at Instituto de Geociências of the Universidade de São Paulo by means of a JEOL JXA-8600 electron microprobe (WDS mode, 15 kV, 20 nA, 10 µm beam diameter) and a Noran system for automation and data reduction. H₂O was inferred from the crystal structure determination. The crystals are unstable under the electron beam but under the selected operational conditions, this instability seems not to affect the chemical analyses. Analytical results are represented in Table 1. No elements with Z > 8, other than those reported herein, were indicated by EDS. Total Fe was partitioned as Fe2+ in the Mg-site (Mg + Fe²⁺ = 1 apfu) and Fe³⁺ in the Al-site (Al + Fe³⁺ approach 5 apfu). This may not be correct, because in natrodufrénite Fe in the site corresponding to Mg is predominantly Fe³⁺. Unfortunately the available material is insufficient for Fe²⁺ and Fe³⁺ discrimination. The empirical formula for matioliite is the following [based on 19 O atoms (anhydrous) and incorporating

 $\begin{array}{l} H_2O \mbox{ and } OH \mbox{ as suitable for the crystal structure]: } (Na_{0.94}Ca_{0.01})_{\Sigma 0.95} \\ (Mg_{0.88}Fe_{0.11}^{2+}Mn_{0.01})_{\Sigma 1.00} \ (Al_{4.84}Fe_{0.13}^{3+})_{\Sigma 4.97} (PO_4)_{4.03} (OH)_{5.76} 0.2 H_2O. \\ The ideal formula is NaMgAl_5 (PO_4)_4 (OH)_6 \cdot 2 H_2O, \mbox{ which yields the following wt% oxide values: } Na_2O = 4.43, \mbox{ MgO} = 5.76, \mbox{ Al}_2O_3 \\ = 36.41, \ P_2O_5 = 40.54, \ H_2O = 12.87, \ Total = 100.00. \end{array}$

TABLE 1. Chemical composition of matioliite from Gentil mine (in wt%)

Constitue	ent 1	1	2	2	standard	Probe
	(range)		(range)		deviation	standard
Na ₂ O	4.07	3.85-4.26	3.88	3.48-4.07	0.1	albite
CaO	0.06	b.d0.14	0.08	0.04-0.17	0.01	anorthite
MgO	4.92	4.13-5.54	2.76	2.34-3.23	0.08	diopside
MnO	0.14	0.03-0.35	0.08	0.05-0.10	0.04	olivine
FeO*	1.10		4.99		0.2	olivine
$Fe_2O_3^*$	1.45		0.55			
AI_2O_3	34.36	33.63-34.95	34.90	34.00-36.70	0.2	chlorapatite
P_2O_5	39.79	38.76-40.67	38.98	38.00-39.91	0.6	GaP
H₂O†	12.19		12.52			
Total	98.08		98.74			

Notes: b.d. = below detection. 1 = matioliite (mean of 17 analyses). 2 = Fe-rich phase with a Fe²⁺:Mg ratio of approximately 1:1, corresponding to an intermediate burangaite-matioliite composition (mean of 7 analyses).

*Total Fe analyzed as FeO: 2.41 wt% (range = 1.43-3.34) for 1, and 5.50 wt% (range = 4.40-5.87) for 2, divided over FeO and Fe₂O₃ to sum 1 apfu in the Mg site. + H₂O calculated for 2 molecules in the formula.

 TABLE 2.
 Powder X-ray diffraction data for matioliite from Gentil mine

I _{meas.}	d _{meas.} (Å)	$d_{\rm calc.}$ (Å)	I _{calc.}	h	k	1
100	11.654	11.707	47	2	0	0
62	6.581	6.600	20	2	0	2
20	5.833	5.854	6	4	0	0
13	4.930	4.934	55	1	1	0
62	4.862	4.854	72	2	0	2
		4.275	13	3	1	1
		4.028	35	1	1	2
15	4.011	4.021	14	6	0	2
		3,879	6		1	2
		3.797	15	3	1	1
		3 743	5	1	1	2
18	3 5 5 3	3 5 5 7	28	5	1	1
10	5.555	3 344	9	2	0	4
23	3,291	3 316	57	3	1	3
14	3 1 3 8	3 1 3 7	35	0	0	4
• •	5.150	3 1 1 3	48	<u> </u>	õ	2
31	3 103	3 1 1 0	4	5	1	1
10	3.075	3 079	100	≚ 5	1	3
12	5.075	3.078	72	1	1	3
40	3 0 2 7	3 031	4	<u>+</u> 6	0	4
12	2 912	2 912	58	27	1	1
12	2.912	2.212	50	6	0	2
		2.005	35	2	1	4
17	2 785	2.7 24	11	7	1	0
17	2.705	2.700	1	<u>/</u>	0	1
-15	2.000	2.005	27	7	1	1
٥	2 5 1 7	2.505	20	,	2	0
2	2.517	2.325	29	2	2	1
		2,500	7	2	1	5
		2.371	6	5	1	2
10	2 3/0	2,300	11	2	0	2
0	2.349	2,330	10	05	1	5
<i>,</i>	2.542	2.555	7	2	2	2
15	2 0/1	2.030	40	<u>_</u>	1	1
7	2.041	2.045	3	1	1	6
/	2.040	2.039	20	2	2	4
		2.014	15	4	2	4
10	1 040	2.004	15	4	2	4
7	1.940	1.942	23	4	2	4
/	1.950	1.959	5 14	6	2	4
		1.099	14	0	2	2
		1.057	5	9	1	4
		1./94	11	5 12	1	/
		1.090	5 14	13	1	0
14	1 (70	1.095	14	13	1	2
14	1.6/8	1.6/8	/	6	0	ŏ
7	1.072	1.072	11	14	U	U

Figure 2 shows a zoned crystal where the darker parts correspond to matioliite and the lighter parts correspond to a Ferich phase with a Fe²⁺:Mg ratio of approximately 1:1.Chemical analyses were done for this phase (Table 1) and the empirical formula is $(Na_{0.90}Ca_{0.01})_{\Sigma0.91}(Fe_{0.50}^{2+}Mg_{0.49}Mn_{0.01})_{\Sigma1.00}(Al_{4.95}Fe_{0.05}^{3+})_{\Sigma5.00}$ (PO₄)_{3.97}(OH)_{6.01}·2H₂O.

CRYSTALLOGRAPHY

Powder X-ray diffraction (XRD) data were obtained with a Siemens D5000 diffractometer equipped with a Göbel mirror and a position-sensitive detector using CuK α radiation and 40 kV and 40 mA at Instituto de Geociências of the Universidade de São Paulo. (Table 2). Observed and calculated relative intensities differ significantly due to preferred orientation. The same discrepancy between observed and calculated patterns occurs with burangaite (ICDD cards 29-1190 and 88-331, respectively

observed and calculated patterns). Matioliite is isostructural with burangaite, dufrénite, and natrodufrénite (Table 3).

A single crystal was selected for intensity measurements on an Enraf-Nonius Kappa-CCD diffractometer using graphitemonochromatized MoK α radiation, at the Instituto de Física de São Carlos, Universidade de São Paulo. The diffraction intensities were measured by the ω -2 θ scan technique. Data collection (φ scans and ω scans with κ offsets) was made using the program COLLECT (Enraf Nonius, Delft, The Netherlands, 1997). Final cell parameters based on all reflections, integration, and scaling of the reflections intensities were performed with the HKL DENZO SCALEPACK system of programs (Otwinowski et al. 1997). The structure was solved using direct methods and refined by full matrix least squares procedure on F^2 with SHELXS-97 (Sheldrick 1997). The crystal-structure data and characteristics of the XRD study are given in Table 4. The values for *R* factors are relatively high when compared to those obtained for burangaite



FIGURE 1. Matioliite aggregate on quartz from Gentil mine, Mendes Pimentel, Minas Gerais, Brazil.



FIGURE 2. Back-scattered electron image of a zoned crystal where the darker parts correspond to matioliite and the lighter parts to a Ferich phase with a Fe²⁺:Mg ratio of approximately 1:1, corresponding to an intermediate burangaite-matioliite composition. A line of spots from EDS is in the center of the figure.

TABLE 3. Comparative data for matioliite and isostructural minerals

	Matioliite*	Burangaite†	Dufrénite‡	Natrodufrénite§
Chemical formula	NaMgAl ₅ (PO ₄) ₄ (OH) ₆ ·2H ₂ O	NaFe ²⁺ Al ₅ (PO ₄) ₄ (OH) ₆ ·2H ₂ O	Ca _{0.5} Fe ²⁺ Fe ³⁺ ₅ (PO ₄) ₄ (OH) ₆ ·2H ₂ O	(Na,)(Fe ³⁺ , Fe ²⁺)(Fe ³⁺ , Al) ₅ (PO ₄) ₄ (OH) ₆ ·2H ₂ O
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	C2/c	C2/c	C2/c	C2/c
Unit-cell	a = 25.075(1) Å	a = 25.099(2) Å	<i>a</i> = 25.84(2) Å	<i>a</i> = 25.83(2) Å
parameters	<i>b</i> = 5.0470(3) Å	<i>b</i> = 5.0491(7) Å	<i>b</i> = 5.126(3) Å	b = 5.150(3) Å
	<i>c</i> = 13.4370(7) Å	<i>c</i> = 13.438(1) Å	<i>c</i> = 13.78(1) Å	<i>c</i> = 13.772(9) Å
	$\beta = 110.97(3)^{\circ}$	$\beta = 110.88(1)^{\circ}$	$\beta = 111.20(6)^{\circ}$	$\beta = 111.50^{\circ}$
Strongest lines	11.747 – 86	11.71 – 100	12.00 – 90	12.04 - 80
in the powder	6.583 – 100	4.86 - 41	5.002 - 90	5.040 - 60
pattern	4.021 – 50	3.318 – 39	3.393 – 70	3.400 - 80
	3.109 - 60	3.115 – 70	3.151 – 100	3.204 - 80
	2.670 – 49	3.081 – 90	2.860 - 60	3.152 – 100
Optical data	$\eta_{\alpha} = 1.597(2)$	$\eta_{\alpha} = 1.611(2)$	$\eta_{\alpha} = 1.810 - 1.842$	$\eta'_{\alpha} = 1.765(5)$
	$\eta_{\beta} = 1.627(2)$	$\eta_{\beta} = 1.635(2)$	$\eta_{\beta} = 1.813 - 1.850$	$\eta_{\beta} = n.d.$
	$\eta_{\gamma} = 1.632(1)$	$\eta_{\gamma} = 1.643(1)$	$\eta_{\gamma} = 1.855 - 1.925$	$\eta'_{\gamma} = 1.775(5)$
	2V = 43(2)°	2V = 58°	2V = small to very small	2V = n.d.

* This work.

† von Knorring et al. (1977); Selway et al. (1997).

‡ Anthony et al. (2000).

§ Fontan et al. (1982).

by Selway et al. (1997), probably due to crystal quality. Matioliite crystals can have portions with different chemical compositions (see Fig. 2). The unit cell is monoclinic, and the space group is C2/c with a = 25.075(1) Å, b = 5.0470(3) Å, c = 13.4370(7) Å, $\beta = 110.97(3)^\circ$, V = 1587.9(4) Å³, Z = 4. The a:b:c ratio calculated from the unit-cell parameters is 4.9683:1:2.6624. Gladstone-Dale compatibility $1 - (K_P/K_C) = 0.020$, excellent. Walter and Ettinger (2001) obtained the following unit-cell parameters for matioliite from Austria: a = 25.06(5) Å, b = 5.057(1) Å, c = 13.44(1) Å, $\beta = 110.92(2)^\circ$.

Atomic coordinates, equivalent isotropic parameters, and anisotropic displacement parameters are represented in Table 5. Selected bond lengths and angles are given in Table 6. Calculated and observed structure factors are provided in Table 7¹.

Like burangaite (Selway et al. 1997), the fundamental building block of the structure of matioliite is a face-sharing triplet of octahedra [Al ϕ_6 -Mg ϕ_6 -Al ϕ_6] corner linked to two Al ϕ_6 octahedra and two PO₄ tetrahedra (ϕ = unspecified anionic species). This block is polymerized parallel to the **c**-axis to form dense slabs in the {100} plane. Alternating Al ϕ_6 octahedra and Na ϕ_8 polyhedra form a chain parallel to the **c**-axis, and the dense slab and chain alternate along the **a**-axis. The Na site is coordinated by six O anions and two (H₂O) groups to form a cubic antiprism. Magnesium is coordinated by four O anions and two (OH) groups in an octahedral arrangement. Aluminum occurs at three symmetrically

¹ Deposit AM-06-031, Table 7. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the American Mineralogist Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there. distinct sites, each coordinated in an octahedral arrangement. The Al1 site is coordinated by two O anions, two (OH) groups and two (H_2O) groups. The Al3 site is coordinated by three O anions and three (OH) groups. The Al4 site is coordinated by

	TABLE 4.	Crystal	data	and	structure	refinemer	۱t
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Temperature	120(2) K
Wavelength	0.71073 Å
Absorption coefficient	1.011 mm ⁻¹
F(000)	931
Crystal size	$0.18 \times 0.15 \times 0.10 \text{ mm}^3$
Theta range for data collection	3.25 to 27.50°
Index ranges	$-32 \le h \le 32, -6 \le k \le 6, -17 \le l \le 17$
Reflections collected	5825
Independent reflections	1795 [<i>R</i> (int) = 0.0919]
Completeness to theta = 27.50°	98.0%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.978 and 0.798
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	1795/0/168
Goodness-of-fit on F ²	1.020
Final R indices $[l>2\sigma(l)]$	<i>R</i> 1 = 0.0535, w <i>R</i> 2 = 0.1264
R indices (all data)	R1 = 0.0741, wR2 = 0.1399
Largest diff. peak and hole	0.715 and –0.675 e.Å ⁻³



TABLE 5. Atomic coordinates (×10⁴), equivalent isotropic and anisotropic displacement parameters ($Å^2 × 10^3$)* for matioliite

	Х	у	Ζ	$U_{\rm eq}$	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Na	0	6488(4)	2500	29(1)	28(1)	28(1)	30(1)	0	11(1)	0
P1	2161(1)	2341(2)	3281(1)	20(1)	25(1)	13(1)	24(1)	0(1)	10(1)	1(1)
P2	807(1)	2245(2)	3951(1)	21(1)	24(1)	15(1)	26(1)	0(1)	10(1)	-1(1)
Mg†	2500	7500	5000	19(3)	19(5)	22(5)	21(5)	0(3)	11(4)	5(3)
Fe†	2500	7500	5000	31(7)	40(12)	5(8)	39(11)	-2(7)	2(8)	-13(6)
Al1	0	5000	5000	22(1)	24(1)	17(1)	28(1)	0(1)	11(1)	-1(1)
Al3	1518(1)	4827(2)	6099(1)	22(1)	24(1)	16(1)	26(1)	-1(1)	10(1)	-1(1)
Al4	1412(1)	7234(2)	3518(1)	20(1)	24(1)	14(1)	24(1)	-1(1)	10(1)	0(1)
01	918(1)	4450(5)	3270(2)	25(1)	31(1)	15(1)	29(1)	-3(1)	13(1)	1(1)
02	805(1)	9559(5)	3422(2)	23(1)	29(1)	14(1)	28(1)	-2(1)	13(1)	-2(1)
03	213(1)	2766(5)	4018(2)	25(1)	25(1)	21(2)	28(1)	-1(1)	10(1)	-3(1)
04	1258(1)	2215(5)	5073(2)	24(1)	27(1)	16(1)	28(1)	1(1)	9(1)	0(1)
05	1683(1)	7154(5)	5098(2)	22(1)	28(1)	16(1)	26(1)	0(1)	12(1)	0(1)
06	2087(1)	4948(5)	3814(2)	23(1)	27(1)	14(1)	28(1)	1(1)	11(1)	-1(1)
07	1972(1)	10002(5)	3826(2)	23(1)	27(1)	16(1)	28(1)	-2(1)	11(1)	2(1)
08	1294(1)	7481(5)	2054(2)	23(1)	26(1)	16(1)	26(1)	-2(1)	9(1)	2(1)
09	1756(1)	12440(5)	2113(2)	24(1)	26(1)	17(1)	28(1)	-1(1)	8(1)	-1(1)
010	2775(1)	11904(5)	3411(2)	26(1)	28(1)	20(1)	31(1)	0(1)	13(1)	-1(1)
011	748(1)	6282(5)	5645(2)	25(1)	27(1)	17(1)	32(1)	-2(1)	11(1)	-4(1)
012	-214(1)	7781(5)	3972(2)	26(1)	26(1)	19(1)	30(1)	-2(1)	9(1)	2(1)
H5	1627	8143	5453	33						
H8	1417	8647	1973	34						
H11	723	7290	6016	38						
H12A	-109	9188	3895	38						
H12B	-618	7643	3588	38						

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor. † Occupancy Mg_{0.9}Fe_{0.1}. 1935

TABLE 6. Selected bond lengths (Å) for matioliite

TABLE O. Sciected Bolia lengtis	(i) for mationic
Na-O1,a	2.391(3)×2
Na-O2,a	2.494(3)×2
Na-O3,a	2.682(3) ×2
Na-O12,a	2.321(3)×2
Mean	2.472
Mg-O5,c	2.105(2) ×2
Mg-O6,c	2.022(2) ×2
Mg-O7,c	2.083(2)×2
Mean	2.070
Al1-011,d	1.877(2)×2
Al1-012,d	1.906(2) ×2
Al1-O3,d	1.950(3) ×2
Mean	1.911
AI3-O4	1.849(3)
AI3-O5	1.939(3)
AI3-O8f	1.958(3)
Al3-O9e	1.880(3)
Al3-O10c	1.872(3)
Al3-011	1.949(3)
Mean	1.908
Al4-O1	1.825(3)
AI4-O2	1.891(3)
AI4-O5	1.984(3)
AI4-06	1.968(3)
Al4-07	1.917(3)
AI4-08	1.887(3)
Mean	1.912
P1-O6	1.541(2)
P1-07b	1.550(2)
P1-O9b	1.535(3)
P1-O10b	1.501(3)
Mean	1.532
P2-O1	1.528(2)
P2-O2b	1.529(3)
P2-O3	1.547(3)
P2-O4	1.527(3)
Maan	1 5 2 2

Note: Symmetry transformations used to generate equivalent atoms: a = -x,y,-z+1/2; b = x,y-1,z; c = -x+1/2,-y+3/2,-z+1; d = -x,-y+1,-z+1; e = x,-y+2,z+1/2; f = x,-y+1,z+1/2.

four O anions and two (OH) groups. Phosphorus occurs at two symmetrically distinct sites, each coordinated in a tetrahedral arrangement (Fig. 3).

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