

JAHNSITE-(MnMnMg), $\text{Mn}^{2+}\text{Mn}^{2+}\text{Mg}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_4(\text{OH})_2 \cdot 8\text{H}_2\text{O}$, A NEW PHOSPHATE MINERAL SPECIES FROM SAPUCAIA PEGMATITE, SAPUCAIA DO NORTE, GALILÉIA, MINAS GERAIS, BRAZIL

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ABSTRACT

Jahnsite-(MnMnMg), $\text{Mn}^{2+}\text{Mn}^{2+}\text{Mg}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_4(\text{OH})_2 \cdot 8\text{H}_2\text{O}$, is a new phosphate mineral belonging to the jahnsite subgroup contained in the jahnsite group of minerals. It was found in the dumps of the Sapucaia pegmatite, Sapucaia do Norte, Galiléia, Minas Gerais, Brazil by one of the authors (SV). The mineral occurs on the surfaces of hydrothermal cavities and is associated with frondelite, mangangordonite, and leucophosphite. It forms prisms weakly elongated along **a**, flattened on [010], and twinned by reflection on {001} up to 200 μm in length. The new species is a late stage alteration product of primary phosphates such as triphylite. Its color is yellow to honey-colored or greenish-yellow and it is partially transparent with a vitreous luster. The streak is very pale yellow. Jahnsite-(MnMnMg) is brittle with good cleavage on {001} and irregular fracture. Its inferred Mohs hardness is 4 and the calculated density is 2.625 g/cm^3 . The mineral is optically biaxial (–) with $\alpha = 1.616$, $\beta = 1.619$, $\gamma = 1.656$ and $2V(\text{calc.}) = 74^\circ$ and non-fluorescent under 254 nm (short wave) and 366 nm (long wave). The empirical formula is: $(\text{Mn}_{0.50}\text{Ca}_{0.25}\text{Na}_{0.20})_{\Sigma 0.95}\text{Mn}(\text{Mg}_{1.26}\text{Mn}_{0.52}\text{Fe}^{2+}_{0.21}\text{Zn}_{0.01})_{\Sigma 2}(\text{Fe}^{3+}_{1.63}\text{Al}_{0.37})_{\Sigma 2}(\text{PO}_4)_4(\text{OH})_{1.70} \cdot 8\text{H}_2\text{O}$. The endmember formula is $\text{Mn}^{2+}\text{Mn}^{2+}\text{Mg}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_4(\text{OH})_2 \cdot 8\text{H}_2\text{O}$. Jahnsite-(MnMnMg) is monoclinic, with space group $P2/a$ and unit-cell parameters a 15.177(2) Å, b 7.176(1) Å, c 10.006(3) Å, and β 110.01(2)° with V 1017.3(2) Å³ for $Z = 2$. Its crystal structure was refined and the mineral is isostructural with other members of the jahnsite group.

Keywords: jahnsite-(MnMnMg), jahnsite group, jahnsite subgroup, new mineral species, pegmatitic phosphate, Sapucaia, Minas Gerais, Brazil.

INTRODUCTION

Jahnsite-group minerals (Kampf *et al.* 2018a) are common secondary phosphates occurring in granitic pegmatites. According to the new nomenclature of the jahnsite group, characterized by the general formula $X\text{M}_1\text{M}_2\text{M}_3\text{M}_4(\text{PO}_4)_4(\text{OH})_2 \cdot 8\text{H}_2\text{O}$, the group can be

divided into the jahnsite subgroup ($\text{M}_3 = \text{Fe}^{3+}$) and the whiteite subgroup ($\text{M}_3 = \text{Al}$) (Kampf *et al.* 2018a). The jahnsite subgroup now consists of 11 different mineral species and this number is in continuous growth thanks to the extremely flexible crystal-chemical features of these phosphates. The species

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belonging to the jahnsite subgroup, as explained in Kampf *et al.* (2018a), have the general formula $XM1M2Fe^{3+}(PO_4)_4(OH)_2 \cdot 8H_2O$, in agreement with the formula of Moore & Ito (1978). The *X* site is generally occupied by the largest cations, whereas the *M1* and *M2* sites are occupied by small cations such as Fe^{2+} , Fe^{3+} , Mn^{2+} , and Mg^{2+} . The crystal structure of “jahnsite” was first described by Moore & Araki (1974) in the monoclinic space group $P2_1/a$, but they reported only isotropic thermal parameters. Subsequently, Kampf *et al.* (2008) described the structure of the new species jahnsite-(NaFeMg) from the Tip Top Mine (South Dakota, U.S.A.) in the same space group, located the protons and gave anisotropic thermal parameters. Jahnsite-group minerals are commonly found as accessory minerals in granitic pegmatites, where they form by hydrothermal alteration of earlier-formed phosphate minerals, both primary and secondary, under relatively oxidizing conditions (Simmons *et al.* 2003, Vignola *et al.* 2011, Vignola 2018).

In this paper we describe the chemical composition, crystal structure, and optical and morphological features of the new species jahnsite-(MnMnMg) from the famous Sapucaia pegmatite. Recently, jahnsite-(NaMnMg) was described from the same locality (Kampf *et al.* 2018b). The new phosphate described in this article, jahnsite-(MnMnMg), and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification IMA2017-118 (Vignola *et al.* 2018). The type sample used for the complete characterization of the new species jahnsite-(MnMnMg) is deposited in the Mineralogical Collection of the Laboratoire de Minéralogie, University of Liège, Belgium (number n° 21140).

OCCURRENCE, GENERAL APPEARANCE, AND PHYSICAL PROPERTIES

Jahnsite-(MnMnMg) was found by one of the authors (SV) in the dumps of the Sapucaia pegmatite, Sapucaia do Norte, Galiléia, Minas Gerais, Brazil (18° 54' 3" S, 41° 29' 4" W). The Sapucaia pegmatite is a complex pegmatitic dike showing five zones as described by Baijot *et al.* (2012). Phosphates occur in the inner wall zone and inner zone of the pegmatite and form two different phosphate mineral associations, association I and association II, depending on the intensity of oxidation of the genetic environment (Baijot *et al.* 2012). Association I displays stronger oxidizing conditions compared to association II and shows the most varied association of phosphates, which are dominated by lipscombite. According to Baijot *et al.* (2012) and Baijot (2016), this association consists mainly of ferrisicklerite, heterosite, variscite, Fe-hydrated phosphates (rockbridgeite, barbosaltite,

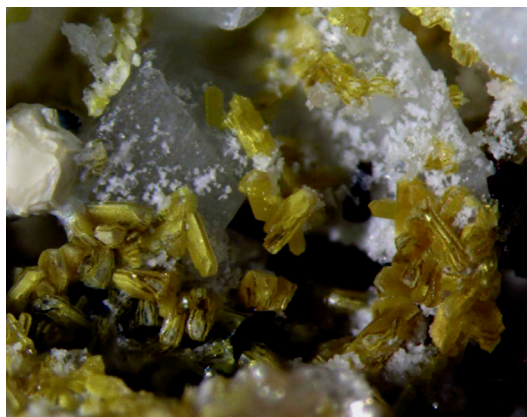


Fig. 1. Prismatic crystals of jahnsite-(MnMnMg) up to 250 μm in size.

phosphosiderite), hureaulite, and minerals belonging to the jahnsite subgroup. The same authors describe jahnsite-(MnMnMg) as an endmember of the series, with jahnsite-(MnMnMg) to jahnsite-(CaMnMg) occurring as rim or intergrowths with ferrisicklerite, or as acicular yellow crystals.

The specimen containing jahnsite-(MnMnMg) described in this work and used for the complete description of the new species was found as single crystals or groups of crystals perched on albite crystals in hydrothermal cavities hosted by a metasomatic unit of the pegmatite composed of large lamellar aggregates of albite var. *cleavelandite*. The new species occurs in close association with frondelite, leucophosphate, and mangangordonite as prisms up to 250 μm in length and elongated on [100], flattened on {010}, and twinned by reflection on {001}. The crystals of jahnsite-(MnMnMg) show a particular indented texture of {001} terminations (Fig. 1). The color is rather variable from yellow to greenish or brownish yellow with a vitreous luster, and the streak is very pale yellow. The hardness could not be measured due to the small size of the crystals, but the Mohs hardness is inferred to be 4 by analogy with the other species belonging to the jahnsite subgroup. Jahnsite-(MnMnMg) is brittle with an irregular fracture and a perfect cleavage on {001}. The density, calculated from the formula weight and single crystal unit-cell parameters, is 2.625 g/cm³. The mineral is optically biaxial negative with $\alpha = 1.616(1)$, $\beta = 1.619(3)$, $\gamma = 1.656(2)$ (sodium light, $\lambda = 589$ nm), and $2V$ (calc.) = 74°, with a strong dispersion $r < v$. The optical orientation is: α is roughly perpendicular to the cleavage (001). The pleochroism is: X = greenish grey; Y = yellow; Z = greenish yellow.

TABLE 1. ELECTRON-MICROPROBE COMPOSITION OF JAHNSITE-(MnMnMg)

Constituent	wt.%	Range	SD
P ₂ O ₅	34.45	(33.44–35.17)	0.67
Al ₂ O ₃	2.31	(0.54–3.13)	1.03
Fe ₂ O ₃ *	15.75		
FeO	1.79 (FeO _{tot} 15.96)	(14.85–16.74)	0.96
MnO	17.41	(15.67–19.79)	1.67
CaO	1.72	(1.49–1.96)	0.19
MgO	6.16	(5.53–6.64)	0.45
ZnO	0.12	(0.03–0.26)	0.09
Na ₂ O	0.77	(0.45–0.95)	0.21
H ₂ O **	19.35		
Total	99.83		

* Calculated to have 2 Fe³⁺ + Al *apfu* at the M³⁺ structural site, ** calculated for 8 H₂O molecules and 1.7 OH *pfu*.

TABLE 3. DATA COLLECTION AND STRUCTURE REFINEMENT DETAILS FOR JAHNSITE-(MnMnMg)

Crystal shape	Irregular prism
Crystal size (μm)	170 × 120 × 100
Crystal color	Pale yellow, transparent
T (K)	298
Unit-cell constants	<i>a</i> = 15.177 (2) Å <i>b</i> = 7.176 (1) Å <i>c</i> = 10.006 (3) Å <i>β</i> = 111.01 (2)° <i>V</i> = 1017.3 (2) Å ³
Reference chemical formula	MnMnMg ₂ Fe ³⁺ ₂ (PO ₄) ₄ (OH) ₂ ·8H ₂ O
Space Group	<i>P2</i> / <i>a</i>
<i>Z</i>	2
Radiation	X-ray MoKα
Wavelength (Å)	0.7107
Diffractionmeter	Xcalibur
Data-collection method	w/φ scan
<i>h</i> _{min} , <i>h</i> _{max}	–24/24
<i>k</i> _{min} , <i>k</i> _{max}	–11/11
<i>l</i> _{min} , <i>l</i> _{max}	–12/12
Redundancy	7.507
Measured reflections	26,229
Unique reflections	2619
Unique refl. with <i>I</i> > 3σ(<i>I</i>)	1703
Parameters (refinement)	208
<i>R</i> _{int}	7.13/8.92
<i>R</i> ₁ (obs/all) (%)	4.04/8.19
Final w <i>R</i> ₂	3.82/4.08
Residuals (e [–] Å ³)	+0.62/–0.85

$$R_{int} = \sum |F^2_{obs} - F^2_{obs}(\text{mean})| / \sum (F^2_{obs}); R_1 = \sum (|F_{obs} - F_{calc}|) / \sum |F_{obs}|;$$

$$wR_2 = (\sum (w(F^2_{obs} - F^2_{calc})^2) / \sum (w(F^2_{obs})^2))^{0.5}, w = 1 / (\sigma^2(F^2_{obs})).$$

TABLE 2. X-RAY POWDER DIFFRACTION DATA FOR JAHNSITE-(MnMnMg) (*d*_{obs}, *d*_{calc} in Å)

<i>l</i> / <i>h</i>	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>l</i> _{calc}	<i>h k l</i>
100	9.282	9.316	100	0 0 1
9	5.727	5.688	15	1 1 1
39	4.945	4.944	18	1 1 1
20	4.627	4.658	19	0 0 2
18	3.984	4.013	22	2 1 1
43	3.521	3.506	25	1 1 2
10	3.266	3.281	27	3 1 1
52	2.988	2.989	30	2 1 3
81	2.842	2.844	50	0 2 2
18	2.601	2.607	35	5 1 0
15	2.355	2.355	20	0 2 3
27	1.958	1.959	15	0 2 4
13	1.882	1.879	6	8 0 2
6	1.783	1.781	1	1 4 0
12	1.739	1.735	1	2 3 3
2	1.662	1.663	1	2 0 5
7	1.581	1.580	1	5 3 2
10	1.530	1.530	4	4 2 4
2	1.340	1.341	1	7 4 0
2	1.297	1.297	1	0 4 5
2	1.251	1.251	1	0 2 7
2	1.216	1.215	1	8 0 4
3	1.178	1.178	0	9 3 2
2	1.164	1.164	0	7 1 5
1	1.024	1.024	0	7 5 3
1	0.988	0.988	0	7 4 5
2	0.964	0.965	0	10 4 3

The Gladstone-Dale compatibility index, calculated from the chemical composition, calculated density, and measured refractive indices, is 0.040, in the “good” category according to Mandarino (1981).

CHEMICAL COMPOSITION

Chemical compositions were obtained from a polished and carbon coated section of jahnsite-(MnMnMg) with a JEOL JXA-8200 electron microprobe working in wavelength-dispersion mode at the laboratory of the Department of Earth Sciences, University of Milan. The system was operated using an accelerating voltage of 15 kV, a beam current of 5 nA, a spot size of 5 μm, and a counting time of 30 s on the peaks and 10 s on the backgrounds. The following minerals were used as standards: graftonite KF16 (Fransolet 1975) for (PKα, FeKα, MnKα, and CaKα), anorthite An 137 for (AlKα), olivine – USNM 2566 for (MgKα), rhodonite for (ZnKα), omphacite USNM 110607 for (NaKα), orthoclase PSU OR 1A for (KKα), and hornblende – Hbl 123 for (Kα). K and F were below the detection limit for all analyzed points.

TABLE 4. REFINED POSITIONAL AND ISOTROPIC THERMAL DISPLACEMENT PARAMETERS (\AA^2) FOR JAHNSITE-(MnMnFe) AT 298 K

Site	Occ	x	y	z	U_{iso}
X	0.752(3)	0.25	0.96792(13)	0	0.0251(5)
Mn(M1)	1	0.25	0.47096(10)	0	0.0204(3)
Mg1(M2)	0.657(3)	0	0	0.5	0.0210(5)
Mg2(M2)	0.634(3)	0.25	0.50252(14)	0.5	0.0195(5)
Fe1(M3)	0.911(3)	0	0	0	0.0161(3)
Fe2(M3)	0.927(3)	0	0.5	0	0.0158(3)
P1	1	0.18375(6)	0.25857(11)	0.18949(11)	0.0179(3)
P2	1	0.08308(6)	0.74765(11)	0.800(11)	0.0187(3)
O1a	1	0.27184(18)	0.2209(4)	0.1498(3)	0.0406(12)
O2a	1	0.21084(19)	0.2991(3)	0.3470(3)	0.0326(11)
O3a	1	0.11932(18)	0.0894(3)	0.1481(3)	0.0420(11)
O4a	1	0.13872(15)	0.4305(3)	0.0914(3)	0.0220(9)
O5a	1	0.18926(17)	0.6906(3)	0.8555(3)	0.0287(10)
O6a	1	0.05200(17)	0.7841(3)	0.6403(3)	0.0268(10)
O7a	1	0.08063(18)	0.9270(3)	0.8855(3)	0.0304(11)
O8a	1	0.02288(17)	0.5922(3)	0.8282(3)	0.0261(10)
Oh	1	0.02584(17)	0.7504(3)	0.0961(3)	0.0231(10)
Ow1	1	0.2258(2)	0.7240(4)	0.3430(3)	0.0369(12)
Ow2	1	0.4489(2)	0.2152(4)	0.3427(3)	0.0421(13)
Ow3	1	0.6316(2)	0.9909(4)	0.4672(4)	0.0403(13)
Ow4	1	0.3935(2)	0.5136(3)	0.5170(3)	0.0363(13)
Hoh	1	1.009(5)	0.749(10)	0.177(5)	0.166(10)
H1a	1	0.253(5)	0.825(7)	0.398(6)	0.166(10)
H1b	1	0.159(2)	0.719(11)	0.291(7)	0.166(10)
H2a	1	0.425(5)	0.300(9)	0.395(7)	0.166(10)
H2b	1	0.396(6)	0.257(10)	0.251(9)	0.166(10)
H3a	1	0.614(6)	-0.004(11)	0.365(3)	0.166(10)
H3b	1	0.582(5)	1.022(10)	0.607(8)	0.166(10)
H4a	1	0.418(4)	0.618(7)	0.487(8)	0.166(10)
H4b	1	0.427(4)	0.450(9)	0.599(5)	0.166(10)
Hx	1	0.666(5)	0.893(8)	0.442(8)	0.166(10)
Hy	1	0.245(5)	0.706(10)	0.263(6)	0.166(10)

Notes: The following elements were used during refinement: Mn at X, Mn at M1, Mg at M2, Fe at M3.

The raw data were corrected for matrix effects using the $\Phi\rho Z$ method from the JEOL series of programs. The averaged (5 point analyses) electron microprobe composition of jahnsite-(MnMnMg) is reported in Table 1. The empirical formula calculated on the basis of 4 P atoms per formula unit is: $(\text{Mn}_{0.50}\text{Ca}_{0.25}\text{Na}_{0.20})_{\Sigma 0.95}\text{Mn}(\text{Mg}_{1.26}\text{Mn}_{0.52}\text{Fe}^{2+}_{0.21}\text{Zn}_{0.01})_{\Sigma 2}(\text{Fe}^{3+}_{1.63}\text{Al}_{0.37})_{\Sigma 2}(\text{PO}_4)_4(\text{OH})_{1.70}\cdot 8\text{H}_2\text{O}$, with H_2O calculated following stoichiometry; charges were balanced by tuning the OH^- content. The cations were distributed at the X, M(1), M(2), and M(3) sites, as suggested by Kampf *et al.* (2018a). The M(3) site is populated by trivalent cations (Fe^{3+} and Al) up to 2 ($\text{Fe}^{3+} + \text{Al}$) *apfu*; M(1) is completely occupied by Mn^{2+} . Site M(2) is filled by the small-sized cations Mg and Zn, the remnant fraction of Fe^{2+} , and the remainder up to 1 *apfu* by Mn^{2+} . The further fraction of Mn^{2+} (0.50 *apfu*) is accommodated at

the X site, together with the large cations Ca and Na, up to a total of 0.95 *apfu*. The simplified formula is $\text{Mn}^{2+}\text{Mn}^{2+}\text{Mg}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_4(\text{OH})_2\cdot 8\text{H}_2\text{O}$, which requires: MnO 17.13 wt.%, MgO 9.73 wt.%, Fe_2O_3 19.28 wt.%, P_2O_5 34.28 wt.%, and H_2O 19.58 wt.%; total 100.00 wt.%.

X-RAY DIFFRACTION DATA AND CRYSTAL STRUCTURE REFINEMENT

The X-ray powder diffraction pattern of jahnsite-(MnMnMg) was collected with an Agilent Xcalibur 4-circle diffractometer, with an EOS CCD detector, using $\text{MoK}\alpha$ radiation (λ 0.71073 \AA) and working in Debye-Scherrer geometry at the Geology Department of the University of Liège, Belgium. Operating conditions were 50 kV, 30 mA, and a sample to detector distance of 40 mm. The very low amount of

TABLE 5. ANISOTROPIC THERMAL PARAMETERS (\AA^2) FOR JAHNSITE-(MnMnMg) AT 298 K

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
X	0.0267(6)	0.0159(5)	0.0257(9)	0	0.0007(5)	0
Mn(M1)	0.0238(4)	0.0183(3)	0.0206(6)	0	0.0099(4)	0
Mg1(M2)	0.0247(6)	0.0187(6)	0.0176(10)	0.0010(4)	0.0052(6)	0.0052(5)
Mg2(M2)	0.0236(7)	0.0189(6)	0.0203(10)	0	0.0103(6)	0
Fe1(M3)	0.0190(4)	0.0108(4)	0.0189(6)	-0.0001(3)	0.0072(4)	0.0003(3)
Fe2(M3)	0.0193(4)	0.0111(3)	0.0185(6)	0.0005(2)	0.0088(4)	0.0005(3)
P1	0.0198(4)	0.0165(4)	0.0171(6)	0.0013(3)	0.0061(4)	-0.0010(4)
P2	0.0212(4)	0.0181(4)	0.0177(7)	0.0025(3)	0.0082(4)	0.0028(4)
O1a	0.0330(15)	0.0659(19)	0.0259(19)	0.0254(14)	0.0143(14)	0.0111(15)
O2a	0.0476(17)	0.0319(14)	0.0177(18)	0.0017(12)	0.0111(14)	-0.0042(12)
O3a	0.0431(16)	0.0173(11)	0.043(2)	-0.0044(11)	-0.0129(15)	0.0048(12)
O4a	0.0224(12)	0.0209(11)	0.0223(17)	0.0006(9)	0.0074(11)	0.0017(11)
O5a	0.0267(13)	0.0356(13)	0.0233(18)	0.0064(11)	0.0083(12)	0.0015(12)
O6a	0.0337(14)	0.0282(13)	0.0161(17)	0.0037(10)	0.0059(12)	0.0047(11)
O7a	0.0449(16)	0.0176(11)	0.036(2)	-0.0025(11)	0.0240(14)	-0.0036(12)
O8a	0.0365(14)	0.0192(11)	0.0283(18)	-0.0030(10)	0.0187(13)	0.0010(11)
Oh	0.0293(13)	0.0153(10)	0.0254(18)	-0.0008(9)	0.0106(12)	-0.0041(11)
Ow1	0.0504(18)	0.0335(15)	0.031(2)	0.0086(13)	0.0189(16)	0.0023(14)
Ow2	0.0562(19)	0.0253(14)	0.029(2)	-0.0038(13)	-0.0041(16)	0.0004(13)
Ow3	0.0414(18)	0.0346(16)	0.050(2)	-0.0044(12)	0.0221(17)	-0.0097(15)
Ow4	0.0305(14)	0.0338(15)	0.045(2)	-0.0021(11)	0.0141(15)	0.0021(14)

specimen was mounted in a glass capillary (70 μm in diameter). Refinement of unit-cell parameters was performed using the program CelRef 3 (Laugier & Bochu 1999), starting from the unit-cell parameters described for jahnsite-(CaMnMg) (jahnsite *auctorum*) by Moore & Araki (1974). The powder pattern reflections were found to be consistent with the space group $P2_1/a$. The refined unit-cell parameters are $a = 14.919(48)$ \AA , $b = 7.145(5)$, $c = 9.927(34)$, $\beta = 110.2(4)^\circ$, $V = 993(10)$. The lower volume obtained by refinement of the powder pattern with respect to that obtained from the crystal structure refinement is due to

the slight imprecision of peak positions induced by peak broadening during the data collection. The complete list of indexed reflections is reported in Table 2.

Single-crystal X-ray diffraction data were obtained from a monocrystalline fragment of jahnsite-(MnMnMg) with an Xcalibur-Oxford Instruments diffractometer equipped with a CCD detector, using graphite-monochromatized $\text{MoK}\alpha$ radiation, and operated at 40 kV and 30 mA at the ESD-MI. Table 3 summarizes the details of the data collection.

TABLE 6. SELECTED BOND DISTANCES (\AA) FOR JAHNSITE-(MnMnMg) AT 298 K

MnX-O3	3.000(3)	$\times 2$	MnM1-O1	2.284(3)	$\times 2$	P1-O1	1.549(3)
MnX-O1	2.302(3)	$\times 2$	MnM1-O4	2.210(3)	$\times 2$	P1-O2	1.507(3)
MnX-O7	2.428(2)	$\times 2$	MnM1-O5	2.114(2)	$\times 2$	P1-O3	1.520(2)
MnX-O5	2.439(3)	$\times 2$	<Mn-O>	2.203		P1-O4	1.572(2)
<Mn-O>	2.542					<P1-O>	1.537
Mg1M2-O6	2.049(2)	$\times 2$	Mg2M2-Ow1	2.171(3)	$\times 2$	P2-O5a	1.559(3)
Mg1M2-Ow2	2.143(3)	$\times 2$	Mg2M2-Ow4	2.124(3)	$\times 2$	P2-O6a	1.519(3)
Mg1M2-Ow3	2.139(3)	$\times 2$	Mg2M2-O2	2.043(3)	$\times 2$	P2-O7a	1.553(3)
<Mg1-O>	2.110		<Mg2-O>	2.113		P2-O8a	1.530(3)
						<P2-O>	1.540
Fe1M3-O7	2.022(3)	$\times 2$	Fe2M3-Oh	2.009(2)	$\times 2$		
Fe1M3-OH	2.004(2)	$\times 2$	Fe2M3-O4	2.034(2)	$\times 2$		
Fe1M3-O3a	1.990(2)	$\times 2$	Fe2M3-O8	1.986(3)	$\times 2$		
<Fe1-O>	2.005		<Fe2-O>	2.010			

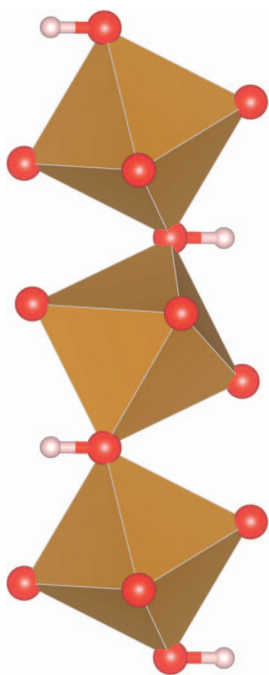


FIG. 2. The $\cdots\text{Fe}^{3+}\text{--OH--Fe}^{3+}\cdots$ octahedral corner-linked chain.

Space group tests led to the $P2_1/a$ space group. The crystal structure of jahnsite-(MnMnMg) was solved using the SUPERFLIP program (based on the charge flipping algorithm, Palatinus & Chapuis 2007) implemented in JANA2006 (Petricek *et al.* 2014), on the basis of the intensity data collected at the ESD-MI. The atomic positions (Table 4) were found to be in good agreement with those described by Kampf *et al.* (2008 and 2018b) for jahnsite-(NaFeMg) and jahnsite-(MnMnZn). We finalized the refinement using anisotropic thermal parameters for the cations (Mn, Mg, Fe, P) and oxygen atoms and isotropic thermal parameters for the H atoms. O–H distances were restrained to 0.95(3) Å. Moreover, thermal parameters for H were constrained to be equal. Only cation occupancies were refined; those for P were close to 1 and ultimately fixed

TABLE 7. SITE-SCATTERING ANALYSIS OF JAHNSITE-(MnMnMg)

Site	Chemical analysis (e^-)	Structure refinement (e^-)	Difference %
X	19.7	18.8	3
M(1)	25	25	0
M(2)	33.98	30.98	9
M(3)	47.19	47.79	1

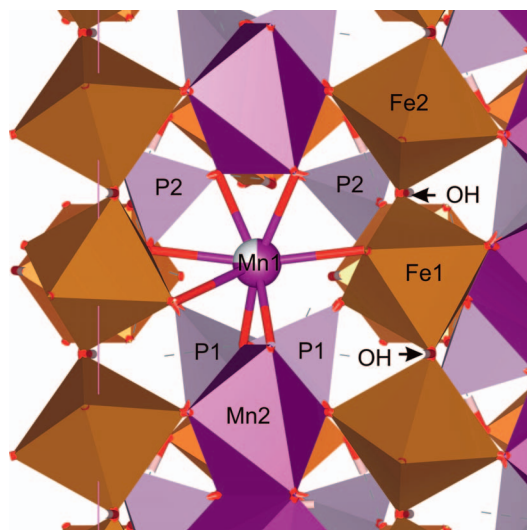


FIG. 3. The $[\text{XM1M3}_2(\text{OH})_2(\text{PO}_4)_4]^{4-}$ slab.

at this value. The other occupancies (O and H) were fixed to full occupancy. When convergence was achieved, no peak larger than +0.62 and $-0.85 \text{ e}^-/\text{\AA}^3$ was present in the final difference-Fourier map. Anisotropic thermal parameters and selected bond distances for jahnsite-(MnMnMg) are given in Tables 5 and 6.

The general framework of jahnsite-(MnMnMg) conforms to that proposed by Moore & Araki (1974) and subsequently by Kampf *et al.* (2008). The jahnsite-(MnMnMg) structure is characterized by a chain of $M3^{3+}$ octahedral sites linked on opposite corners *via* OH anions (Fig 2). As described in Kampf *et al.* (2008), the chains are linked together through perpendicular dense slabs with composition $[\text{XM1M3}_2(\text{OH})_2(\text{PO}_4)_4]^{4-}$ parallel to $\{001\}$ with, in our case, $X = \text{Mn}^{2+}$, $M1 = \text{Mn}^{2+}$, and $M3 = \text{Fe}^{3+}$ (Fig. 3). The complete structure is shown in Figure 4.

DISCUSSION

The mineral is named jahnsite-(MnMnMg), since it corresponds to the MnMnMg member of the jahnsite subgroup, jahnsite group, in which Mn is the principal element at the X site and the unique element at the $M(1)^{2+}$ site. Mg^{2+} predominates at the $M(2)^{2+}$ site. Fe^{3+} represents the main element at the $M(3)^{3+}$ site. This cation distribution is confirmed by the site-scattering analysis represented in Table 7. The e^- densities from the structural refinement and calculated from the distribution of the cations are comparable. The slight difference of e^- density at the M(2) site could be balanced by moving some Fe from M(2) to

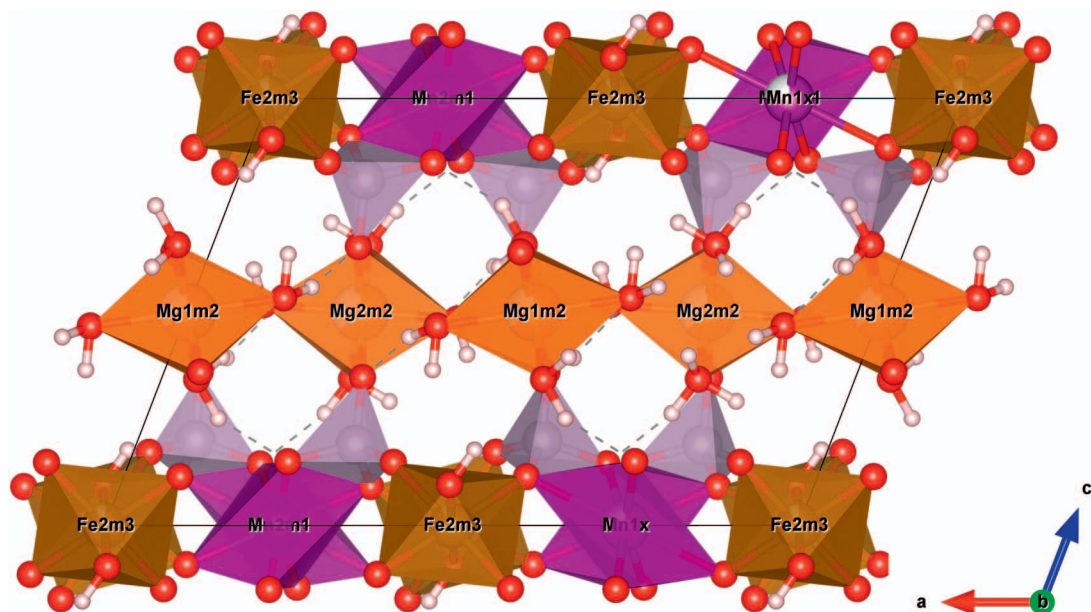


FIG. 4. The crystal structure of jahnsite-(MnMnMg) viewed down *b*.

M(3). The bond valence of ions for jahnsite-(MnMnMg), calculated as in Brown (1996), confirms the charge balance and, further, the cation distribution for the *M*1, *M*2, and *M*3 sites, whereas the *X* site appears to be “under-bonded” due to the two Mn1–O3 distances resulting in a contribution to the valence value of 0.042 × 2, as well as the presence of 0.2 *apfu* of Na at the site (Tables 1, 6, and 8). Due to the lack of

hydrogen atoms in the refinement, the Oh and Ow atoms show a deficit in the electrostatic value. The Dana classification is 42.11.02, hydrated phosphates containing hydroxyl or halogen. The Strunz classification 8.DH.15, phosphates with additional anions (OH[−]) and H₂O, with large- and medium-sized cations. The crystal-structure of jahnsite-(MnMnMg) conforms very well with other jahnsites (Kampf *et al.* 2018b and

TABLE 8. BOND VALENCE FOR JAHNSITE-(MnMnMg)

	Mn1(×2)*	Mn2(×2)	Mg1(×2)	Mg2(×2)	Fe3(×2)	Fe4(×2)	P1	P2	Sum of charges
O1	0.279	0.263					1.202		1.716
O2				0.388			1.346		1.734
O3	0.042				0.536		1.300		1.874
O4		0.321				0.476	1.129		1.926
O5	0.192	0.417						1.170	1.760
O6			0.382					1.303	1.685
O7	0.198				0.491			1.189	1.858
O8						0.541		1.265	1.806
OH**					0.516	0.509			1.025
Ow1**				0.275					0.275
Ow2**			0.296						0.296
Ow3**			0.300						0.300
Ow4**				0.312					0.312
Sum of charges	1.422	2.002	1.956	1.950	3.086	3.052	4.977	4.927	

* The deficit in the charge is due to the strong distortion of the *X* site polyhedron; ** the deficit in the charge is due to the lack of hydrogen atoms in the refinement.

references therein). As happens in jahnsite-(MnMnFe) (Vignola *et al.* 2019), the *X* site in jahnsite-(MnMnMg) appears more deformed with respect to the same site in jahnsite-(NaMnMg) as described by Kampf *et al.* (2018b).

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