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WHITEITE-(CaMgMg), $CaMg_3Al_2(PO_4)_4(OH)_2{\cdot}8H_2O$, A NEW JAHNSITE-GROUP MINERAL FROM THE NORTHERN BELLE MINE, CANDELARIA, NEVADA, U.S.A.

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ABSTRACT

Whiteite-(CaMgMg), $CaMg_3Al_2(PO_4)_4(OH)_2{\cdot}8H_2O$, is a new mineral from the Northern Belle mine, Candelaria, Nevada, U.S.A. It is a low temperature, secondary mineral presumed to have formed as a result of hydrothermal alteration. It is associated with crandallite, fluorwavellite, montgomeryite, and variscite/metavariscite. The mineral occurs as colorless tapering blades, elongated parallel to [100], flattened on {001} and exhibiting the forms {100}, {010}, {001}, $\{11\bar{1}\}$, and $\{13\bar{1}\}$. The streak is white, the luster is vitreous, and crystals are transparent. The Mohs hardness is about 4. The tenacity is brittle, the fracture is irregular and stepped, and there is one perfect cleavage on {001}. The measured density is 2.48(1) g/cm^3. The mineral is very slowly soluble in dilute HCl and slowly soluble in concentrated HCl. Whiteite-(CaMgMg) is biaxial (+), with $\alpha = 1.564(1)$, $\beta = 1.565(1)$, $\gamma = 1.575(1)$ (white light). The measured $2V$ is 24(1)°. No dispersion or pleochroism were observed. The optical orientation is $X = \mathbf{b}$; $Z \wedge \mathbf{a} = 41°$ in obtuse β. Electron-microprobe analyses gave the empirical formula $Ca_{1.07}Mg_{2.99}Fe_{0.01}Al_{1.91}P_4O_{26}H_{18.11}$. The mineral is monoclinic, space group $P2/a$, with unit-cell parameters a 14.8237(19), b 7.0302(3), c 9.946(3) Å, β 110.115(12)°, V 973.3(3) Å^3, and $Z = 2$. The five strongest lines in the X-ray powder diffraction patterns are [d_{obs} Å(I)(hkl)]: 9.20(82)(001), 4.88(64)(210,$21\bar{1}$,111), 2.936(40)(401), 2.849(45)($40\bar{3}$), and 2.805(100)(022). The structure ($R_1 = 4.36\%$ for 1401 reflections with $F_o > 4\sigma F$) is the same as that of other jahnsite-group minerals.

Keywords: whiteite-(CaMgMg), new mineral, jahnsite group, crystal structure, Raman spectroscopy, infrared spectroscopy, electron microprobe analysis, Northern Belle mine, Candelaria, Nevada, U.S.A.

INTRODUCTION

Jahnsite, $CaMnMg_2Fe^{3+}{}_2(PO_4)_4(OH)_2{\cdot}8H_2O$, was first described by Moore (1974) and its crystal structure was determined by Moore & Araki (1974). Moore & Ito (1978) recognized that a variety of cation substitutions were possible in the jahnsite structure type, for which they gave the general formula $XM1M2_2M3_2(H_2O)_8OH)_2(PO_4)_4$, where the X site accommodates the largest cations, the $M1$ and $M2$ sites accommodate medium- to small-sized octahedrally coordinated cations (*e.g.*, Mn^{2+}, Fe^{2+}, Fe^{3+}, and Mg^{2+}), and the $M3$ site accommodates the small octahedrally coordinated cations Fe^{3+} or Al^{3+}. They proposed a naming scheme in which the root name jahnsite is applied to minerals with $M3 = Fe^{3+}$ and whiteite to those with $M3 = Al^{3+}$; the root name is then followed by a suffix of the form -($XM1M2$). They referred to these minerals as comprising the "jahnsite-whiteite complex series". This clearly corresponds to a mineral group as defined by Mills *et al.* (2009). Subsequent workers have referred to this as the

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TABLE 1. MEMBERS OF THE JAHNSITE GROUP*

Species Name	Site assignments X	M1	M2	M3	Reference
Jahnsite subgroup					
Jahnsite-(CaMnMn)	Ca^{2+}	Mn^{2+}	Mn^{2+}	Fe^{3+}	Grice *et al*. (1990)
Jahnsite-(CaMnMg)	Ca^{2+}	Mn^{2+}	Mg^{2+}	Fe^{3+}	Moore (1974), Moore & Ito (1978)
Jahnsite-(CaMnFe)	Ca^{2+}	Mn^{2+}	Fe^{2+}	Fe^{3+}	Moore & Ito (1978)
Keckite	Ca^{2+}	Mn^{2+}	Fe^{3+}	Fe^{3+}	Hochleitner & Fehr (2010)
Jahnsite-(CaFeMg)	Ca^{2+}	Fe^{2+}	Mg^{2+}	Fe^{3+}	Elliott (2016a)
Jahnsite-(MnMnMn)	Mn^{2+}	Mn^{2+}	Mn^{2+}	Fe^{3+}	Moore & Ito (1978)
Jahnsite-(NaFeMg)	Na^{+}	Fe^{3+}	Mg^{2+}	Fe^{3+}	Kampf *et al*. (2008)
Whiteite subgroup					
Whiteite-(CaMnMn)	Ca^{2+}	Mn^{2+}	Mn^{2+}	Al^{3+}	Grey *et al*. (2010), Yakovenchuk *et al*. (2012)
Whiteite-(CaMnMg)	Ca^{2+}	Mn^{2+}	Mg^{2+}	Al^{3+}	Grice *et al*. (1989)
Whiteite-(CaMgMg)	Ca^{2+}	Mg^{2+}	Mg^{2+}	Al^{3+}	This study
Whiteite-(CaFeMg)	Ca^{2+}	Fe^{2+}	Mg^{2+}	Al^{3+}	Moore & Ito (1978), Capitelli *et al*. (2011)
Whiteite-(MnMnMg)	Mn^{2+}	Mn^{2+}	Mg^{2+}	Al^{3+}	Elliott (2016b)
Rittmannite	Mn^{2+}	Mn^{2+}	Fe^{2+}	Al^{3+}	Marzoni Fecia Di Cossato *et al*. (1989)
Whiteite-(MnFeMg)	Mn^{2+}	Fe^{2+}	Mg^{2+}	Al^{3+}	Moore & Ito (1978)

* Several species mentioned in the literature, but never approved by the IMA, are not included.

whiteite group, the whiteite-jahnsite group, or the jahnsite-whiteite group; however, as noted by Mills *et al*. (2009), the group name should generally be that of the first mineral in the group to be adequately characterized; hence, this should be referred to as the jahnsite group. A listing of all currently approved minerals in this group is provided in Table 1. Note that the minerals keckite and rittmannite do not conform to the naming scheme proposed by Moore & Ito (1978).

The name of the new jahnsite-group mineral described herein, whiteite-(CaMgMg), is in accord with the aforementioned naming scheme. The whiteite root name signifies that the M3 site is occupied by Al^{3+} and the suffix is based upon the dominance of Ca at the X site and Mg at both the M1 and M2 sites. The new mineral and name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2016-001). Two cotype specimens are housed in the collections of the Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, California 90007, USA, catalogue numbers 65642 and 65643.

OCCURRENCE AND PARAGENESIS

Whiteite-(CaMgMg) was found at the Northern Belle mine (also known as Argentum mine), Candelaria district, Mineral County, Nevada, USA (38°9′22″N 118°5′8″W). The Northern Belle mine was historically one of the largest silver mines in the area. It was located in 1864, but did not become a significant producer until 1875. The town of Candelaria was developed largely as a result of the success of the Northern Belle mine. In 1884, the Northern Belle was sold to the Argentum Mining Company, which consolidated it with the Holmes mine to create the Argentum mine. The bonanza ores were exhausted in the early 1890s and the district began a decline until production essentially ceased by the mid-1920s. Candelaria is now a ghost town. In spite of the earlier consolidation of the mines, Page (1959) notes that "strictly speaking the Northern Belle mine did not go out of existence". In 1983, the Northern Belle/Argentum mine and nearby Mt. Diablo mine were reopened as open pits (Moeller 1988) which were decommissioned in 1997. Details of the history and geology of the mine and the Candelaria district as a whole are provided by Knopf (1922), Page (1959), Shamberger (1978), and Moeller (1983).

The economic ore mineralization was limited to mineralized fault zones recognizable on the surface as limonite-stained outcrops of fault breccia. Primary ore consisted mainly of pyrite and sphalerite and minor galena, chalcopyrite, and arsenopyrite in a gangue of altered country rock, quartz, and dolomite. Oxidized ore, most of which was mined in the early days, was composed predominantly of limonite and manganese oxide with small amounts of "bindheimite", anglesite, smithsonite, and cerussite. Page (1959) notes veinlets of turquoise and variscite that are found cutting across shale beds in the lower portion of the Candelaria

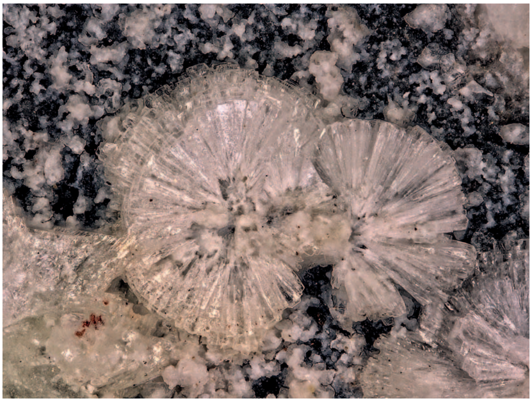

FIG. 1. Radial fans of whiteite-(CaMgMg) blades with montgomeryite (lower left). The FOV is 1.7 mm across.

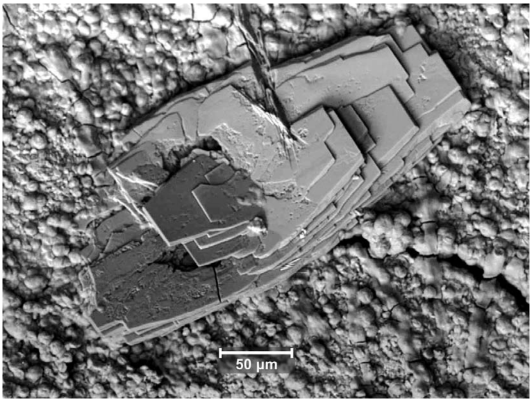

FIG. 2. SEM image of a whiteite-(CaMgMg) blade.

Formation, about 100 feet west of the glory hole at the discovery vein. He further notes that this part of the formation contains ellipsoidal phosphatic nodules and suggests that the phosphate is derived from the sediments.

Whiteite-(CaMgMg) was collected by one of the authors (PMA) from blocks containing hydrothermally altered phosphate nodules (lower Candelaria Formation) in a berm placed to block access to the Northern Belle pit and in a graded area adjacent to the berm. These altered phosphate nodules appear to correspond to those noted by Page (1959). Whiteite-(CaMgMg) has not been found *in situ*. The mineral occurs in seams in dark-colored massive quartz with embedded pyrite. Other secondary species observed in direct association with whiteite-(CaMgMg) are crandallite, fluorwavellite, montgomeryite, and variscite/metavariscite. Other secondary phases in the same general assemblage include collinsite, gordonite, overite, and whitlockite. Whiteite-(CaMgMg) is a low temperature, secondary mineral presumed to have formed as a result of hydrothermal alteration. A major serpentinite body in proximity to the deposit shows evidence of intense hydrothermal alteration, and this is believed to be the source of the Mg in the secondary phases, including whiteite-(CaMgMg).

TABLE 2. ANALYTICAL DATA (wt.%) FOR WHITEITE-(CaMgMg)

Constituent	Mean	Range	SD	Standard
CaO	8.18	7.78–8.64	0.26	diopside
MgO	16.47	15.94–17.05	0.43	diopside
FeO	0.13	0.12–0.16	0.02	hematite
Al_2O_3	13.35	13.11–13.60	0.20	sanidine
P_2O_5	38.84	38.24–39.69	0.45	apatite
H_2O*	22.32			
Total	99.29			

* Based on the crystal structure

PHYSICAL AND OPTICAL PROPERTIES

Whiteite-(CaMgMg) occurs as colorless tapering blades, elongated parallel to [100] and flattened on {001}, commonly forming radial fans on fracture surfaces (Figs. 1 and 2). Crystals exhibit the forms {100}, {010}, {001}, $\{11\bar{1}\}$, and $\{13\bar{1}\}$ (Fig. 3). Twinning by reflection on {001} is common. The streak is white, the luster is vitreous, and crystals are transparent. No fluorescence was observed under SW

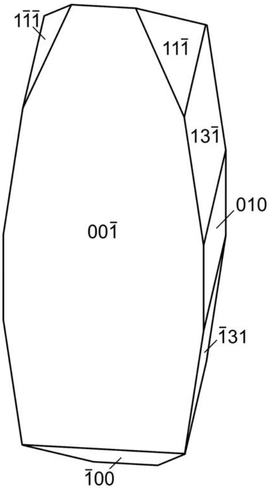

FIG. 3. Crystal drawing of whiteite-(CaMgMg); clinographic projection in non-standard orientation, {100} vertical.

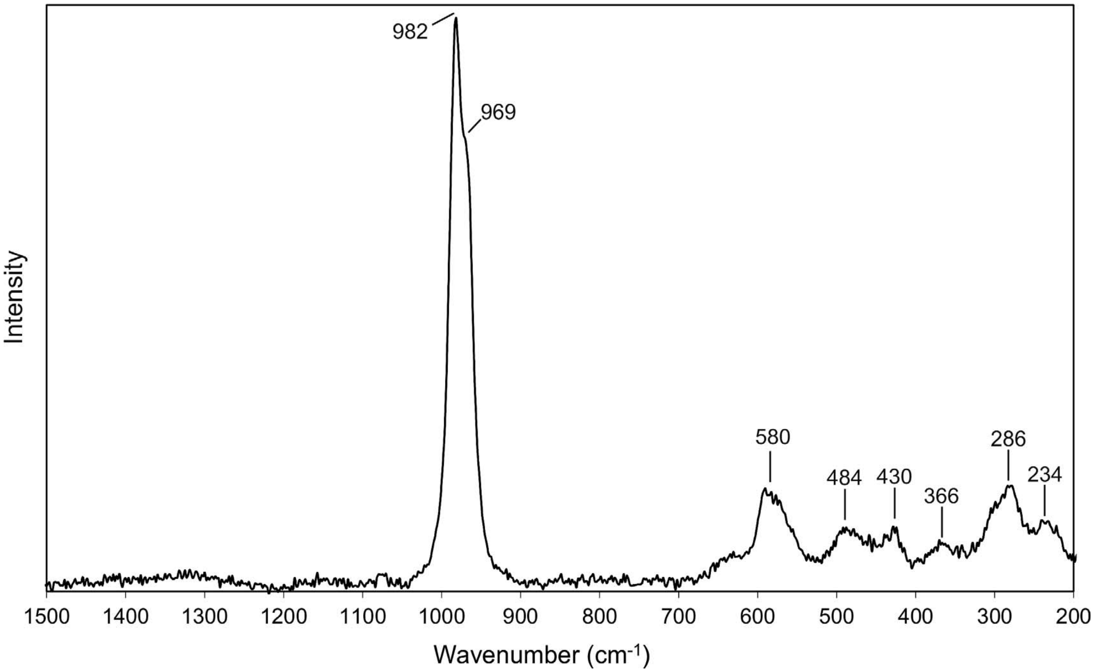

FIG. 4. Raman spectrum of whiteite-(CaMgMg).

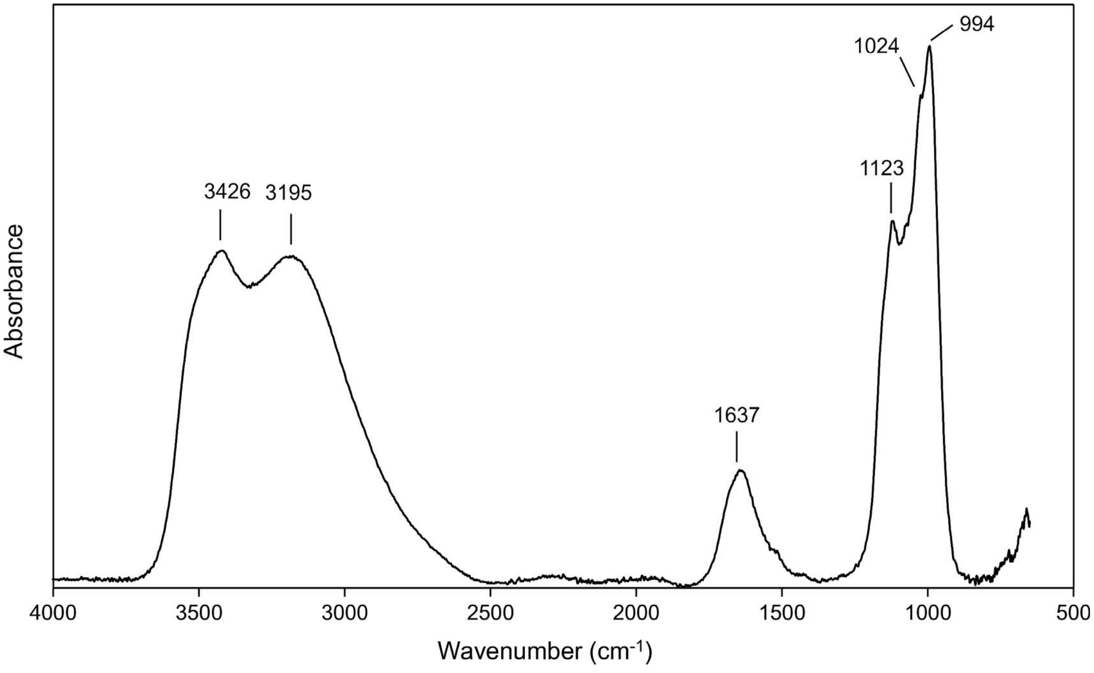

FIG. 5. FTIR spectrum of whiteite-(CaMgMg).

TABLE 3. POWDER X-RAY DIFFRACTION DATA (*d* IN Å) FOR WHITEITE-(CaMgMg)

I_{obs}	d_{obs}	d_{calc}	I_{calc}	*hkl*
82	9.20	9.3393	94	0 0 1
4	6.24	6.2752	6	1 1 0
26	5.62	5.6283	25	1 1 $\bar{1}$
64	4.88	4.9460	9	2 1 0
		4.8934	12	2 1 $\bar{1}$
		4.8708	40	1 1 1
13	4.70	4.6697	12	0 0 2
17	4.059	4.0598	14	1 1 $\bar{2}$
		4.0072	3	3 1 $\bar{1}$
		3.9865	3	2 1 1
22	3.886	3.8725	16	3 1 0
6	3.724	3.7042	8	4 0 $\bar{1}$
35	3.510	3.5180	24	3 1 $\bar{2}$
		3.4957	3	1 1 2
28	3.432	3.4799	13	4 0 0
		3.4078	13	4 0 $\bar{2}$
18	3.260	3.2613	18	3 1 1
		3.1376	2	2 2 0
		3.1241	3	2 2 $\bar{1}$
10	3.106	3.1182	2	1 2 1
		3.1131	6	0 0 3
40	2.936	2.9462	34	4 0 1
45	2.849	2.8598	35	4 0 $\bar{3}$
		2.8441	2	2 2 1
		2.8141	2	2 2 $\bar{2}$
100	2.805	2.8084	100	0 2 2
		2.6517	3	5 1 $\bar{2}$
8	2.614	2.6311	4	1 1 3
		2.5884	8	5 1 0
34	2.549	2.5498	29	4 2 $\bar{1}$
		2.4354	2	2 2 2
6	2.409	2.4037	3	5 1 $\bar{3}$
		2.4014	2	1 2 $\bar{3}$
		2.3482	3	4 0 $\bar{4}$
		2.3441	2	2 1 $\bar{4}$
29	2.309	2.3202	10	6 1 $\bar{1}$
		2.3084	4	1 1 $\bar{4}$
		2.3038	6	6 1 $\bar{2}$
		2.2718	3	6 0 $\bar{3}$
		2.1443	2	3 1 3
11	2.080	2.0917	3	3 3 0
		2.0896	2	6 0 1
		2.0852	5	1 1 4
		2.0563	4	2 2 3
26	2.0045	2.0300	5	3 3 $\bar{2}$
		2.0257	2	1 3 2
		2.0143	2	6 2 $\bar{1}$
		2.0085	2	5 2 1
		2.0030	9	4 0 3
		1.9932	9	4 2 2
		1.9769	4	3 3 1
35	1.9527	1.9526	11	4 2 $\bar{4}$
		1.9485	6	4 0 $\bar{5}$
		1.9449	19	0 2 4
14	1.9217	1.9253	4	2 3 2
		1.9098	5	2 3 $\bar{3}$
		1.9083	3	2 1 $\bar{5}$
28	1.8472	1.8521	22	8 0 $\bar{2}$
2	1.8002	1.8068	4	1 3 3
17	1.7491	1.7576	16	0 4 0
		1.7403	4	4 2 3
		1.7276	2	1 4 $\bar{1}$
5	1.7044	1.7042	5	4 2 $\bar{5}$
4	1.6386	1.6449	2	0 4 2
		1.6339	2	7 1 $\bar{5}$
34	1.5562	1.5688	3	4 4 0
		1.5620	3	4 4 $\bar{2}$
		1.5594	16	8 2 0
		1.5566	7	0 0 6
16	1.5246	1.5332	8	8 2 $\bar{4}$
		1.5222	8	4 2 4
13	1.4954	1.5094	5	4 4 1
		1.4974	4	4 4 $\bar{3}$
		1.4919	10	4 2 $\bar{6}$

Only calculated lines with intensities ≥ 2 are included.

TABLE 4. DATA COLLECTION AND STRUCTURE REFINEMENT DETAILS FOR WHITEITE-(CaMgMg)

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation / power	Mo*K*a (λ = 0.71075 Å) / 50 kV, 40 mA
Temperature	293(2) K
Structural Formula	$Ca(Mg_{2.69}Ca_{0.31})_{\Sigma 3.00}Al_2(PO_4)_4(OH)_2{\cdot}8H_2O$
Space group	*P*2/*a*
Unit cell dimensions	*a* = 14.8237(19) Å *b* = 7.0302(3) Å *c* = 9.946(3) Å β = 110.115(12)°
V	973.3(3) $Å^3$
Z	2
Density (for above formula)	2.491 g/cm^3
Absorption coefficient	1.046 mm^{-1}
F(000)	741
Crystal size	110 × 60 × 10 μm
θ range	3.25 to 25.01°
Index ranges	$-16 \leq h \leq 17$, $-8 \leq k \leq 8$, $-11 \leq l \leq 11$
Reflections collected / unique	7089 / 1703 [R_{int} = 0.040]
Reflections with $F_o > 4\sigma F$	1402
Completeness to θ = 25.01°	98.60%
Min. and max. transmission	0.867 and 0.987
Refinement method	Full-matrix least-squares on F^2
Parameters refined / restraints	197 / 13
GoF	1.075
Final *R* indices [$F_o > 4\sigma F$]	R_1 = 0.0436, wR_2 = 0.1070
R indices (all data)	R_1 = 0.0555, wR_2 = 0.1149
Largest diff. peak / hole	+0.72 / –0.50 *e*/A^3

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})|/\Sigma[F_o^2]$. GoF $= S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where *a* is 0.0504, *b* is 3.2430, and *P* is $[2F_c^2 + \text{Max}(F_o^2,0)]/3$.

or LW ultraviolet radiation. The Mohs hardness is about 4. The tenacity is brittle, the fracture is irregular and stepped, and there is one perfect cleavage on {001}. The density measured by flotation in an aqueous solution of sodium polytungstate is 2.48(1) g/cm^3; the calculated density based on the empirical formula is 2.477 g/cm^3. At room temperature, the mineral is insoluble in H_2O, very slowly soluble in dilute HCl (hours), and slowly soluble in concentrated HCl (minutes).

Whiteite-(CaMgMg) is biaxial (+), with α = 1.564(1), β = 1.565(1), γ = 1.575(1) (measured in white light). The 2*V* measured using extinction data analyzed with the program EXCALIBR (Gunter *et al.* 2004) is 24(1)°; the calculated 2*V* is 35.3°. No dispersion or pleochroism were observed. The optical orientation is *X* = **b**; *Z* ^ **a** = 41° in obtuse β.

RAMAN AND INFRARED SPECTROSCOPY

The Raman spectrum of whiteite-(CaMgMg) was recorded with a Renishaw inVia microprobe using a 785 nm diode laser in order to reduce fluorescence observed with the 514 nm laser. The nominal analysis area was 5 × 50 μm. The FTIR spectrum was recorded with a micro diamond compression cell in transmission mode using a Thermo Nicolet model 6700 spectrometer equipped with a Continuμm microscope.

The Raman and FTIR spectra for whiteite-(CaMgMg) are shown in Figures 4 and 5, respectively. Band assignments were made according to Frost *et al.* (2014). The Raman spectrum shows peaks (in cm^{-1}) at 982, 969 (ν_1 PO_4 symmetric stretch); 580 (ν_4 PO_4 asymmetric bend); 484, 430 (ν_2 PO_4 and H_2PO_4 bending modes); and 366, 286, and 234 (metal–oxygen stretch). The ν_3 PO_4 antisymmetric stretch vibrations at 1173 and 1076 reported by Frost *et al.* (2014) for whiteite-(CaMnMg) and on the RRUFF website (Lafuente *et al.* 2015) for whiteite-(CaFeMg) are very weak. The FTIR spectrum has a broad peak at 3426 from (OH) stretch and a broad band at 3195 from H_2O stretch. The H_2O bending mode was observed at 1637 along with the ν_3 (PO_4) antisymmetric and ν_1 (PO_4) symmetric stretch modes at 1123, 1024, and 994, respectively.

CHEMICAL COMPOSITION

Chemical analyses (seven points on two crystals) were carried out using a Cameca SX-50 electron microprobe in the Department of Geology and Geophysics at the University of Utah (WDS mode, 15 kV, 10 nA, 10 μm beam diameter) utilizing Probe for EPMA software. Raw X-ray intensities were corrected for matrix effects with a $\phi(\rho z)$ algorithm (Pouchou & Pichoir 1991). There was insufficient material for CHN analysis; consequently, we calculated H_2O on the basis of P = 4, charge balance, and 26 O *apfu*, as determined by the crystal-structure analysis (see below). Analytical data are given in Table 2.

The empirical formula (based on 26 O *apfu*) is $Ca_{1.07}Mg_{2.99}Fe_{0.01}Al_{1.91}P_4O_{26}H_{18.11}$. The ideal formula is $CaMg_3Al_2(PO_4)_4(OH)_2{\cdot}8H_2O$, which requires CaO 7.74, MgO 16.68, Al_2O_3 14.06, P_2O_5 39.16, H_2O 22.36, total 100 wt.%. The Gladstone-Dale compatibility index (Mandarino 2007) $1 - (K_P/K_C)$ is –0.012 (superior).

TABLE 5. ATOM COORDINATES AND DISPLACEMENT PARAMETERS (Å^2) FOR WHITEITE-(CaMgMg)

Site	x/a	y/b	z/c	U_{eq}	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca (*X*)	0.25	0.97701(17)	0	0.0231(3)	0.0235(7)	0.0164(6)	0.0234(7)	0.000	0.0003(5)	0
Mg1 (*M*1)*	0.25	0.4798(2)	0	0.0164(7)	0.0241(10)	0.0125(9)	0.0152(10)	0.000	0.0100(7)	0
Mg2 (*M*2)	0.5	0	0.5	0.0160(4)	0.0164(10)	0.0139(9)	0.0154(10)	–0.0039(7)	0.0027(8)	–0.0001(7)
Mg3 (*M*2)	0.25	0.4934(2)	0.5	0.0145(4)	0.0152(9)	0.0143(9)	0.0146(10)	0.000	0.0060(8)	0
Al1 (*M*3)	0	0	0	0.0053(3)	0.0052(7)	0.0036(7)	0.0060(8)	–0.0005(5)	0.0005(6)	0.0004(5)
Al2 (*M*3)	0	0.5	0	0.0047(3)	0.0046(7)	0.0032(7)	0.0065(8)	0.0012(5)	0.0023(6)	0.0007(5)
P1	0.18174(7)	0.26353(14)	0.18641(11)	0.0147(3)	0.0123(5)	0.0147(5)	0.0141(6)	–0.0042(4)	0.0006(4)	0.0024(4)
P2	0.08028(7)	0.74723(13)	0.79971(11)	0.0134(3)	0.0154(5)	0.0130(5)	0.0119(6)	0.0017(4)	0.0049(4)	0.0036(4)
O1	0.2760(2)	0.2424(4)	0.1525(3)	0.0224(7)	0.0190(16)	0.0292(16)	0.0192(16)	0.0025(13)	0.0068(13)	0.0105(12)
O2	0.2026(2)	0.2956(4)	0.3442(3)	0.0228(7)	0.0258(16)	0.0224(15)	0.0204(17)	–0.0070(13)	0.0082(13)	–0.0037(12)
O3	0.1225(2)	0.0829(4)	0.1353(3)	0.0256(7)	0.0276(17)	0.0129(14)	0.0248(17)	–0.0005(12)	–0.0058(13)	–0.0007(12)
O4	0.13406(19)	0.4375(4)	0.0905(3)	0.0219(7)	0.0127(14)	0.0134(13)	0.0336(18)	–0.0033(13)	0.0005(12)	0.0012(11)
O5	0.1883(2)	0.6987(5)	0.8559(3)	0.0268(7)	0.0181(16)	0.0357(17)	0.0218(17)	–0.0078(14)	0.0005(12)	0.0089(13)
O6	0.0465(2)	0.7779(4)	0.6400(3)	0.0197(7)	0.0258(16)	0.0164(14)	0.0139(15)	0.0032(12)	0.0028(12)	0.0024(11)
O7	0.07179(19)	0.9308(4)	0.8794(3)	0.0188(6)	0.0235(15)	0.0143(14)	0.0232(16)	–0.0016(12)	0.0141(13)	0.0002(11)
O8	0.0234(2)	0.5850(4)	0.8345(3)	0.0278(8)	0.050(2)	0.0141(14)	0.0272(18)	–0.0032(13)	0.0239(15)	–0.0051(14)
OH9	0.0228(2)	0.7503(4)	0.0830(3)	0.0146(6)	0.0195(15)	0.0105(13)	0.0152(15)	–0.0006(11)	0.0078(12)	–0.0010(10)
H9	0.001(3)	0.742(7)	0.143(4)	0.022						
OW10	0.2235(3)	0.7168(5)	0.3453(4)	0.0314(8)	0.044(2)	0.0288(17)	0.0227(18)	0.0069(15)	0.0134(16)	0.0165(16)
H10a	0.167(2)	0.739(7)	0.296(5)	0.038						
H10b	0.249(3)	0.709(8)	0.282(5)	0.038						
OW11	0.4525(3)	0.2106(4)	0.3456(4)	0.0334(9)	0.044(2)	0.0183(16)	0.0217(18)	–0.0011(14)	–0.0097(15)	–0.0049(14)
H11a	0.446(4)	0.301(6)	0.392(5)	0.040						
H11b	0.404(3)	0.222(7)	0.271(4)	0.040						
OW12	0.6320(2)	–0.0033(5)	0.4672(4)	0.0324(8)	0.0257(19)	0.0303(19)	0.043(2)	–0.0119(16)	0.0141(16)	–0.0024(14)
H12a	0.658(4)	0.007(7)	0.551(3)	0.039						
H12b	0.653(4)	–0.089(6)	0.433(5)	0.039						
OW13	0.3905(2)	0.5095(4)	0.5080(4)	0.0250(7)	0.0183(16)	0.0255(17)	0.032(2)	0.0107(14)	0.0103(14)	0.0002(12)
H13a	0.432(3)	0.477(6)	0.575(4)	0.030						
H13b	0.408(3)	0.593(6)	0.468(4)	0.030						

* Refined occupancy: 0.691(16) Mg, 0.309(16) Ca.

TABLE 6. SELECTED BOND DISTANCES (Å) AND ANGLES (°) IN WHITEITE-(CaMgMg)

Ca–O1(×2)	2.351(3)	Mg2–O6(×2)	2.048(3)	Al1–OH9(×2)	1.920(3)	P1–O2	1.508(3)
Ca–O5(×2)	2.412(3)	Mg2–OW11(×2)	2.074(3)	Al1–O7(×2)	1.920(3)	P1–O3	1.528(3)
Ca–O7(×2)	2.519(3)	Mg2–OW12(×2)	2.091(3)	Al1–O3(×2)	1.941(3)	P1–O1	1.553(3)
Ca–O3(×2)	2.772(3)	<Mg2–O>	2.076	<Al1–O>	1.928	P1–O4	1.563(3)
<Ca–O3>	2.514					<P1–O>	1.538
		Mg3–O2(×2)	2.020(3)	Al2–O8(×2)	1.892(3)		
Mg1–O5(×2)	2.087(3)	Mg3–OW13(×2)	2.059(3)	Al2–OH9(×2)	1.924(3)	P2–O6	1.508(3)
Mg1–O1(×2)	2.198(3)	Mg3–OW10(×2)	2.139(3)	Al2–O4(×2)	1.929(3)	P2–O8	1.527(3)
Mg1–O4×2)	2.217(3)	<Mg3–O>	2.083	<Al2–O>	1.920	P2–O5	1.542(3)
<Mg1–O>	2.183					P2–O7	1.542(3)
						<P2–O>	1.530

Hydrogen bonds

<*D*–H–*A*	*D*–H···*A*	*D*–H	H···*A*	*D*···*A*
OH9–H9···OW11	0.77(3)	2.39(3)	3.139(5)	16465)
OW10–H10a···OH9	0.82(3)	2.44(4)	3.221(5)	158(5)
OW10–H10b···O5	0.84(3)	1.90(3)	2.744(5)	177(5)
OW11–H11a···OW13	0.81(3)	2.19(3)	2.982(5)	164(5)
OW11–H11b···O1	0.84(3)	1.86(3)	2.670(4)	160(6)
OW12–H12a···OW10	0.79(3)	2.548(5)	3.062(5)	120(5)
OW12–H12b···O2	0.80(3)	1.97(3)	2.774(5)	178(6)
OW13–H13a···O8	0.77(3)	2.50(3)	3.236(5)	158(5)
OW13–H13b···O6	0.80(3)	1.95(3)	2.746(4)	174(5)

TABLE 7. BOND-VALENCE ANALYSIS FOR WHITEITE-(CaMgMg)

	Ca	Al1	Al2	Mg1	Mg2	Mg3	P1	P2	Hydrogen bonds	Σ
O1	0.35 $^{\times 2\downarrow}$			0.34 $^{\times 2\downarrow}$			1.19		+0.24	2.12
O2						0.41 $^{\times 2\downarrow}$	1.34		+0.19	1.94
O3	0.11 $^{\times 2\downarrow}$	0.42 $^{\times 2\downarrow}$					1.27			1.80
O4			0.43 $^{\times 2\downarrow}$	0.33 $^{\times 2\downarrow}$			1.16			1.92
O5	0.30 $^{\times 2\downarrow}$			0.46 $^{\times 2\downarrow}$				1.22	+0.21	2.19
O6					0.38 $^{\times 2\downarrow}$			1.34	+0.21	1.93
O7	0.22 $^{\times 2\downarrow}$	0.44 $^{\times 2\downarrow}$						1.22		1.88
O8			0.48 $^{\times 2\downarrow}$					1.28	+0.10	1.86
OH9		0.44 $^{\times 2\downarrow}$	0.44 $^{\times 2\downarrow}$						–0.11, +0.10	0.87
OW10						0.30 $^{\times 2\downarrow}$			–0.10, –0.21, +0.12	0.11
OW11					0.36 $^{\times 2\downarrow}$				–0.13, –0.24, +0.11	0.10
OW12					0.34 $^{\times 2\downarrow}$				–0.12, –0.19	0.03
OW13						0.37 $^{\times 2\downarrow}$			–0.10, –0.21, +0.13	0.19
Σ	1.96	2.60	2.70	2.26	2.16	2.17	4.96	5.06		

Note: Multiplicity is indicated by ×2↓. P^{5+}–O and Al–O bond-valence parameters are from Brese & O'Keeffe (1991). Ca–O and Mg–O are from Brown & Altermatt (1985). Hydrogen-bond strengths based on O–O bond lengths from Ferraris & Ivaldi (1988). Values are expressed in valence units.

X-ray Crystallography and Structure Refinement

Both powder and single-crystal X-ray studies were done using a Rigaku R-Axis Rapid II curved imaging-plate microdiffractometer with monochromatized Mo$K\alpha$ radiation. A polycrystalline sample was used for the powder-diffraction study; a Gandolfi-like motion on the φ and ω axes was used to further randomize the sample. Observed *d*-values and intensities were derived by profile fitting using JADE 2010 software. Data are given in Table 3. Unit-cell parameters refined from the powder data using JADE 2010 with whole pattern fitting are *a* 14.852(12), *b* 7.053(12), *c* 9.979(12) Å, β 110.17(2)°, and $V = 981(2)$ Å^3.

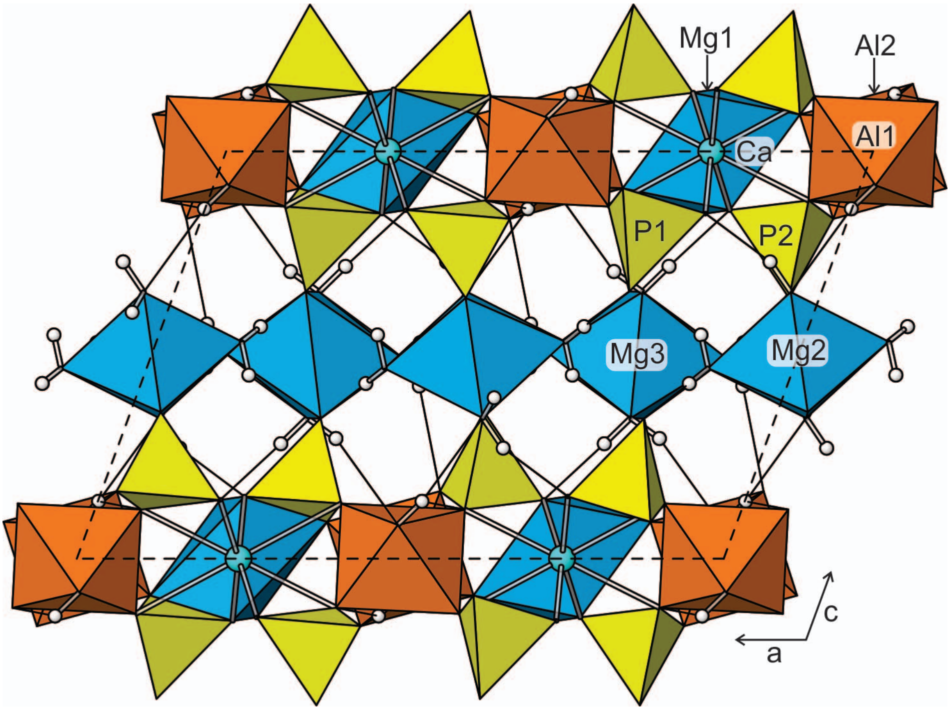

FIG. 6. The structure of whiteite-(CaMgMg) viewed along [010]. Ca–O and O–H bonds are thick black lines; H···O (hydrogen) bonds are thin black lines. The unit-cell outline is dashed.

An untwinned crystal fragment was used for the structure refinement. The Rigaku CrystalClear software package was used for processing of structure data, including the application of an empirical multiscan absorption correction using ABSCOR (Higashi 2001). SHELXL-97 software (Sheldrick 2008) was used for the refinement of the structure. The starting atom coordinates for the structure refinement were taken from the structure determination of jahnsite-(NaFeMg) by Kampf *et al*. (2008). Difference-Fourier syntheses located all H atom sites, which were then refined with soft restraints of 0.82(3) Å on the O–H distances and 1.30(3) Å on the H–H distances and with the U_{eq} of each H tied to that of its O atom (×1.5 for OH and ×1.2 for H_2O). Details of data collection and structure refinement are provided in Table 4. Fractional coordinates and atom displacement parameters are provided in Table 5, selected interatomic distances in Table 6, and bond valences in Table 7. Tables of observed and calculated structure-factors are available from the Depository of Unpublished data on the Mineralogical Association of Canada website [document whiteite-(CaMgMg) CM54-6_10.3749/canmin.1600051].

Whiteite-(CaMgMg) is isostructural with other members of the jahnsite group, which have the general formula $XM1M2_2M3_2(PO_4)_4(OH)_2\cdot 8H_2O$. The $M2$ and $M3$ sites each correspond to two nonequivalent, but structurally similar, sites. In whiteite-(CaMgMg), $X =$ Ca, $M1 =$ Mg1, $M2 =$ Mg2 and Mg3, and $M3 =$ Al1 and Al2. The structure is based on a chain of $M3^{3+}$ octahedra linked by sharing *trans*-OH corners with one another and further linked by sharing corners of PO_4 tetrahedra decorating the chains. The structure possesses dense slabs of $[XM1M3_2(OH)_2(PO_4)_4]^{4-}$ oriented parallel to {001}, which are bridged by PO_4 corner-sharing to $M2\text{-}(O,H_2O)_6$ octahedra (Fig. 6).

There have been several structure refinements of jahnsite-group minerals (see Table 1), which have included detailed discussions of the general structure, individual cation coordinations, and hydrogen bonding. The structure of whiteite-(CaMgMg) closely corresponds to those earlier determinations, so further discussion of the structure seems unwarranted here.

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